

Effective equations for isotropic quantum cosmology including matter

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Abstract

Effective equations often provide powerful tools to develop a systematic understanding of detailed properties of a quantum system. This is especially helpful in quantum cosmology where several conceptual and technical difficulties associated with the full quantum equations can be avoided in this way. Here, effective equations for Wheeler–DeWitt and loop quantizations of spatially flat, isotropic cosmological models sourced by a massive or interacting scalar are derived and studied. The resulting systems are remarkably different from that given for a free, massless scalar. This has implications for the coherence of evolving states and the realization of a bounce in loop quantum cosmology.

1 Introduction

While initial stages of the expanding branch of our universe are becoming better and better understood, its potential history before the big bang remains open to many debates. By now, several scenarios have been suggested which, building on quantum gravity effects rather than purely classical gravity, could give rise to a non-singular evolution at all times [1, 2, 3, 4, 5, 6]. The era preceding the classical big bang singularity, as well as the quantum transition through it, can then be relevant to explain observed features of our universe and must therefore be thoroughly understood. Most of these scenarios realize the simplest possible non-singular behavior where an isotropic collapsing universe reaches a smallest,

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non-zero volume before it bounces back into an expanding branch. In addition to isotropy, one often assumes a special form of matter, such as a free massless scalar making quantum cosmological models solvable. Whether or not this results in a robust, reliable scenario for a complex universe can only be seen by embedding such simple models in a more general class, at least perturbatively, including matter interactions or inhomogeneities. From a conceptual viewpoint, this provides a stability analysis of the original model; from a phenomenological viewpoint it will allow one to construct realistic scenarios with all ingredients relevant for observations.

Loop quantum cosmology gives rise to a potentially general mechanism which removes space-time singularities [7, 8, 9]. In this general form, not much is said about the precise regime around the big bang and the state before, and especially at, the classical singularity might have been highly quantum. This, in fact, agrees with general expectations. It thus came as quite a surprise when detailed properties derived for an isotropic model in loop quantum cosmology sourced by a free, massless scalar indicated that the state remained semiclassical to a high degree throughout its evolution, before and after the big bang [10]. This model was analyzed because the absence of a potential allows a direct calculation of observables and an implementation of the physical inner product. This, in turn, made it possible to evaluate numerical solutions to the underlying evolution equations for physical information [11, 12]. When such special mathematical simplifications, beyond those already implied by assuming space-time symmetries, are used it is never clear whether detailed properties are general or specific to the chosen model. This especially applies to the semiclassical aspects which were unexpected from the point of view of general quantum systems whose states usually spread. An analytical analysis of a related and exactly solvable model¹ [14, 15] clarified this issue and showed that the semiclassicality properties were indeed very special: the bounce is described by a solvable model in which expectation values and fluctuations (or higher moments of a wave function) do not couple to each other. Thus, while the state evolves, its expectation values are not affected by its spreading, and the spreading is completely independent of other parameters of the state. In other words, the system is analogous to a harmonic oscillator in quantum mechanics whose states can remain coherent forever while following the classical trajectory. As quantum systems go, this high degree of solvability is a rare property well-known from the harmonic oscillator or free quantum field theories but not corresponding to a general feature.

In this model, expectation values, spread parameters and higher moments of a state evolve independently of each other and can be determined exactly. Thus, while the wave function evolves and possibly spreads and deforms, this does not influence the trajectory followed by its expectation values. But when details of the model are changed, solvability can no longer be maintained and complicated coupling terms between expectation values,

¹Solvability requires one to drop some of the ingredients of a loop quantized Hamiltonian which, however, are not relevant for states of a universe with large matter content. The solvable model is thus not exactly the same as a loop quantization or that used in the numerical studies of [11] but still allows one to analyze the bounce. Note that also in [11] the dynamical equation was adapted for the numerical purposes and differs from what one would obtain in a loop quantization [13]. None of these changes matter for properties of the bounce of a large universe.

spreads and higher moments arise. This leads to quantum corrections to the classical equations which can often be captured in effective equations [16, 17, 18]. In this paper, we set out to study such effective equations for an isotropic model in loop quantum gravity with a *massive and self-interacting* scalar in order to test the genericness of properties of the exactly solvable model. While the solvability of the exact bounce model certainly makes its properties very special, it also provides the starting point for a systematic perturbation analysis. This is analogous to free field theories used as the zeroth order in perturbative quantum field theory. Adding a potential as done here is the simplest generalization in that it does not introduce additional degrees of freedom. (Initial steps to include inhomogeneities have been done in [19].) However, it also leads to difficulties since the scalar, instead of being a monotonic function of coordinate time as in the free case, has itself non-trivial dynamics. As discussed in more detail below, a monotonic scalar is used crucially in the solvable model since evolution of the universe volume is described relationally with respect to the scalar. If the scalar is no longer monotonic, it cannot be used as a global time coordinate, meaning that the model with a potential can only be used for a finite range of time. Nevertheless, we will see that this allows one to test whether quantum back-reaction effects remain negligible or whether they can have a strong effect on the behavior of a bounce.

It is often assumed that a potential term of a scalar field cannot have a sizable effect near an isotropic classical singularity because its classical form $a^3V(\phi)$ tends to zero for $a \rightarrow 0$ while the kinetic term $\frac{1}{2}a^{-3}p_\phi^2$ in canonical variables has a diverging pre-factor. The general behavior certainly depends also on how p_ϕ and ϕ behave when the singularity is approached, but if the potential is small p_ϕ does not change much, being a constant of motion in the free case. Thus, the kinetic term is expected to dominate and a non-zero potential should not change much of the bounce observed in free models. However, this reasoning overlooks the quantum nature of the problem. It is based on a classical Hamiltonian and the evolution equations it implies. If quantum gravity is used to argue for the free bounce, quantum aspects must also be taken into account for interactions implied by the potential. Here, details of the free bounce related to solvability become important. The solvable bounce model demonstrates that a state which starts out semiclassically at large volume and evolves to smaller volume stays semiclassical and then, *in this semiclassical form*, bounces when quantum geometry effects set in. The model also shows that there do exist states, though not semiclassical ones, which do not bounce [15]. This does not alter the conclusions about singularity removal in the free model since one always has to use the boundary condition that a state is semiclassical at large volume (at least at one side of the bounce). Under this condition, every solution of the free model bounces. But this is no longer guaranteed with interacting matter. Any realistic statement about singularity removal has to involve evolution over long stretches of time: a universe which is semiclassical at large volume, like our own, must be shown to remain non-singular after a long time of backward (or forward) evolution. This does not play a large role for a solvable model since there are no quantum back-reaction effects of an evolving state on its expectation values. But a non-zero potential introduces such back-reaction effects which must be considered even if they are small for a perturbative potential. A reliable statement

about non-singular behavior must involve a proof that a state starting out semiclassically at large volume does not spread and deform too much so as to avoid a bounce, which may well be possible since the free model allows non-semiclassical states which do not bounce. In general, the bounce regime, or whatever regime is valid around the classical big bang singularity, is expected to be of a highly quantum nature; arguments based solely on states which are semiclassical in this regime, by choice or by the lack of quantum back-reaction in a specific model, cannot be complete.

In this paper, we provide effective equations taking into account quantum back-reaction in the presence of a perturbative potential and provide an initial investigation. This is a first step of a stability analysis of bounce models in loop quantum cosmology. We will find several new properties and arrive at a set of effective equations of a new type requiring the presence of independent quantum degrees of freedom. Even though by construction we need to require the potential to be small and a perturbation to the kinetic term, several new qualitative features can be seen. The analytical, though approximate, analysis allows more general conclusions than numerical investigations, which are often prone to hidden assumptions, would show.

2 Description of the models

We start with the Friedmann equation in an isotropic and homogeneous background with a scalar field ϕ . It can be written as a constraint $C = 0$ with

$$C = -\frac{3}{8\pi G}c^2\sqrt{|p|} + \frac{1}{2}|p|^{-3/2}p_\phi^2 + |p|^{3/2}V(\phi), \quad (1)$$

in terms of canonical variables $|p| = a^2$, $c = da/d\tau$ (using proper time τ) for the metric and $p_\phi = a^3 d\phi/d\tau$ as the canonical momentum conjugate to ϕ . We will be ignoring factors of $8\pi G/3$ in this article to keep subsequent formulas simple. A convenient understanding of dimensions then is to use dimensionless c and ϕ while p and $1/V$ have the dimension of length squared. Also the Planck constant \hbar has the dimension of length squared if G is ignored in $\hbar G = \ell_P^2$ with the Planck length ℓ_P . The variable p is derived from an isotropic densitized triad [20] and can thus in general assume both signs to take into account the triad orientation. In this paper, however, it will be sufficient to use only positive values of p since our aim is to analyze bounces; a change of sign in p would imply that no bounce occurs. (Even if quantum effects imply regular evolution through the classical singularity at $p = 0$, this would not be considered a bounce which conventionally requires a non-zero lower bound to volume. “Bounce” is usually also reserved for situations in which a semiclassical description remains valid at all times and the universe does not enter a deep quantum regime. This is realized in all examples for bounces described so far.)

The Friedmann equation describes the dynamics of an isotropic space-time

$$ds^2 = -d\tau^2 + a(\tau)^2(dx^2 + dy^2 + dz^2)$$

with the scale factor a , sourced by a homogeneous scalar matter field with potential $V(\phi)$. Since (1) is a constraint, it generates equations of motion by $df/dt = \{f, NC\}$ for any

phase space function f , referring to a derivative by a time coordinate t which corresponds to the chosen lapse function N . For proper time τ , as in the above line element, we simply have $N = 1$. Then,

$$dp/d\tau = 2\sqrt{|p|}c \quad (2)$$

$$dc/d\tau = -\frac{c^2}{2\sqrt{|p|}} - \frac{3}{2|p|} \left(\frac{p_\phi^2}{2|p|^{3/2}} - |p|^3 V(\phi) \right) \quad (3)$$

$$d\phi/d\tau = |p|^{-3/2} p_\phi \quad (4)$$

$$dp_\phi/d\tau = -|p|^{3/2} V'(\phi). \quad (5)$$

The first and third equation determine the relation between momenta and time derivatives of coordinates, while the other two then result in second order evolution equations for p and ϕ in proper time.

2.1 Internal time

Instead of using a coordinate time τ , we can solve (1) for p_ϕ ,

$$\frac{1}{\sqrt{2}}|p_\phi| = |p|\sqrt{c^2 - |p|V(\phi)} =: H \quad (6)$$

and view the right hand side as a Hamiltonian generating relational evolution in ϕ . Rather than solving for $p(\tau)$, $c(\tau)$ and $\phi(\tau)$ where, due to general covariance the choice of time coordinate τ does not matter, we thus eliminate coordinate time altogether and look for solutions $p(\phi)$ and $c(\phi)$. We will deal here mainly with a perturbative scheme considering the potential to be small in comparison with the gravitational contribution. Thus, we will often refer to the expanded Hamiltonian

$$H = |p|c - \frac{p^2}{2c} V(\phi) + O(V^2) \quad (7)$$

up to second order in V .

Relational solutions in terms of ϕ can easily be found explicitly in the potential free case since p_ϕ is a constant and thus ϕ is a monotonic function of τ . Any point in τ is mapped one-to-one to a value of ϕ . However, if there is a non-trivial potential such as a mass term $\frac{1}{2}m^2\phi^2$, in general ϕ will no longer be monotonic but shows oscillations around minima of the potential. Only stretches between two turning points of ϕ can then be described in an internal time form, but not all of the evolution that would be accessible in τ . Moreover, the system is more complicated due to an explicit “time” dependence from $V(\phi)$ appearing in H . As we will see, upon quantization this still allows us to investigate the effects of spreading and deforming wave packets on the expectation values of a corresponding quantum system. In particular, interesting phases in early universe cosmology are inflationary which, if sourced by an inflaton, typically provides a slow-roll phase where the scalar rolls down a flat potential. In fact, we will see shortly that the potential we deal

with perturbatively must be flat so as to provide this setting automatically. This implies a long monotonic phase for ϕ during which back-reaction effects could build up and become important. In backward evolution, this allows us to see if quantum effects could possibly prevent or dramatically change a bounce.

2.2 Wheeler–DeWitt quantization

A further difficulty related to the potential arises at the quantum level. To see this we first recall from [14] how the potential-free case is treated quantum theoretically. Instead of a time dependent Hamiltonian, this case would give us simply $\frac{1}{\sqrt{2}}|p_\phi| = |pc|$ which, when quantized, results in a Schrödinger equation

$$i\hbar \frac{1}{\sqrt{2}} \frac{\partial}{\partial \phi} \psi = \widehat{|pc|} \psi. \quad (8)$$

Solutions to this equation automatically solve the equation

$$-\frac{\hbar^2}{2} \frac{\partial^2}{\partial \phi^2} \psi = \widehat{p^2 c^2} \psi \quad (9)$$

which (in a certain factor ordering) quantizes (1) before taking the square root. Since the Friedmann equation, from the canonical point of view, is the Hamiltonian constraint, it is indeed quantized first without solving for p_ϕ in canonical quantum gravity. Although (9) is a second order differential equation and thus has more solutions than the first order equation (8), one usually allows superpositions only of solutions with a fixed sign of energy p_ϕ which is chosen positive in taking the root above. Thus, the solution space to (9) relevant for the quantum theory should be considered as consisting of two sectors, one of which is given by solutions to (8) and the other by solutions with the opposite sign of the square root.

A solvable model is then obtained by using the Hamiltonian $\hat{H} = \frac{1}{2}(\hat{c}\hat{p} + \hat{p}\hat{c})$ for ϕ -evolution which is quadratic in canonical coordinates, just as the harmonic oscillator Hamiltonian. This is responsible for the solvability, a fact which, more surprisingly, even extends to the loop quantization [14] as recalled in the next subsection. Solvability implies that the equations of motion (written in internal time ϕ whose derivative is denoted by a dot)

$$\langle \dot{\hat{p}} \rangle = \frac{\langle [\hat{p}, \hat{H}] \rangle}{i\hbar} = -\langle \hat{c} \rangle \quad , \quad \langle \dot{\hat{c}} \rangle = \frac{\langle [\hat{c}, \hat{H}] \rangle}{i\hbar} = \langle \hat{p} \rangle \quad (10)$$

form a closed system and can thus be solved easily without knowing the complicated ways a state may spread and deform. In general quantum systems, by contrast, such equations would form a system of infinitely many coupled equations also involving the quantum variables

$$G^{a,n} = \langle ((\hat{c} - \langle \hat{c} \rangle)^{n-a} (\hat{p} - \langle \hat{p} \rangle)^a)_{\text{Weyl}} \rangle \quad (11)$$

for $2 \leq n \in \mathbb{N}$ and $0 \leq a \leq n$ [16, 17], the subscript “Weyl” denoting fully symmetric ordering. Strictly speaking, this is even the case in the system considered here since we

dropped the absolute value of the Hamiltonian to make it quadratic. As discussed in detail in [15], the quadratic constraint still allows one to describe states correctly which are sharply peaked at large values of energy H or p_ϕ , a case of primary interest for isotropic cosmological models. For the quadratic Hamiltonian, explicit solutions to (10) for expectation values $c = \langle \hat{c} \rangle$ and $p = \langle \hat{p} \rangle$ as well as fluctuations are given by

$$c_{V=0}(\phi) = C_1 e^\phi \quad (12)$$

$$p_{V=0}(\phi) = C_2 e^{-\phi} \quad (13)$$

$$G_{V=0}^{cc}(\phi) = C_3 e^{2\phi} \quad (14)$$

$$G_{V=0}^{cp}(\phi) = C_4 \quad (15)$$

$$G_{V=0}^{pp}(\phi) = C_5 e^{-2\phi} \quad (16)$$

which we distinguish from the perturbative solutions with non-vanishing potential determined later by the subscript. Since to the orders analyzed here we are mainly interested in fluctuations, we will use only quantum variables at $n = 2$, and call them $G^{cc} := G^{0,2}$, $G^{cp} := G^{1,2}$ and $G^{pp} := G^{2,2}$ for better clarity.

In the presence of a potential we would, following the same procedure, first quantize to obtain a second order equation

$$-\frac{\hbar^2}{2} \frac{\partial^2}{\partial \phi^2} \psi = \left(\widehat{p^2 c^2} - |\hat{p}|^3 V(\phi) \right) \psi. \quad (17)$$

Now, however, $[\hat{p}_\phi, \hat{H}] \neq 0$ for a quantization of

$$H = |p| \sqrt{c^2 - |p| V(\phi)}. \quad (18)$$

Thus, solutions to

$$-\frac{1}{\sqrt{2}} \hat{p}_\phi \psi = \hat{H} \psi \quad (19)$$

do not solve the second order equation (17) but rather

$$\frac{1}{2} \hat{p}_\phi^2 \psi = \hat{p}_\phi \hat{H} \psi = \hat{H} \hat{p}_\phi \psi + [\hat{p}_\phi, \hat{H}] \psi = \hat{H}^2 \psi + [\hat{p}_\phi, \hat{H}] \psi. \quad (20)$$

There is thus no strict analog of the first order equation, complicating any analysis.

However, for the solutions we are interested in here, which includes perturbations around solutions of the exact free scalar model obtained for large H , we can ignore the commutator term. In fact, due to the square root in \hat{H} we have, up to factor ordering in a precise quantization,

$$[\hat{p}_\phi, \hat{H}] \sim i\hbar \frac{|\hat{p}^3| V'(\phi)}{2\hat{H}}$$

whose expectation value is small compared to that of \hat{H}^2 , also appearing in (20) for states with large H and a not too steep potential. This is exactly the regime we intend to probe

by our perturbation theory. Such a regime easily arises without fine-tuning and can thus provide general insights: The two conditions $|p|^3 V(\phi) \ll p^2 c^2 \approx H^2$ for the potential term to be perturbative and $\hbar p^3 V'(\phi)/H \ll H^2$ for the commutator in (20) to be negligible require $V \ll H^2/p^3$ and $\hbar V' \ll H^3/p^3$. In the loop quantized model to be discussed next, a semiclassical bounce in the free model occurs for $H \gg \hbar$ for the universe not to enter the deep quantum regime, and we have $p \geq H$. Thus, around such a bounce the conditions on the potential are $\hbar V \ll 1$ and $\hbar V' \ll 1$, such that both the potential and its first derivative must be small compared to the Planck mass squared. For a sufficiently small and flat potential, long evolution times can be considered. For the purpose of describing those regimes, the first order equation (19) is a good approximation, and due to large p_ϕ we can again drop absolute values on H .

2.3 Loop quantization

It is more interesting to study perturbations around the solvable model determined by a loop Hamiltonian following again [14] for the zeroth order solutions. In a loop quantization there is no operator for c [21], and one can thus not use a Hamiltonian of the same form as before. Instead, all exponentials $e^{i\alpha c}$ with $\alpha \in \mathbb{R}$ are represented by well-defined operators and appear in the Hamiltonian such that the classical expression cp is reproduced in the classical, small-curvature limit. This is accomplished by the free Hamiltonian $p \sin c$ as it follows from the loop quantization (up to quantization choices which we can ignore here). This Hamiltonian is no longer quadratic in the canonical variables and one could thus expect strong quantum back-reaction even in the free model. However, this turns out not to be the case since one can choose non-canonical variables p together with $J = pe^{ic}$ in which the system becomes linear: We have classical Poisson relations

$$\{p, J\}_{\text{class}} = -iJ \quad , \quad \{p, \bar{J}\}_{\text{class}} = i\bar{J} \quad , \quad \{J, \bar{J}\}_{\text{class}} = 2ip. \quad (21)$$

Moreover, the Hamiltonian $H = \frac{1}{2i}(J - \bar{J})$ is a linear combination of the basic variables, making the dynamical system (p, J, H) a linear one. For such systems, if they remain linear after quantization, no quantum back-reaction occurs. (A quadratic Hamiltonian in canonical variables is a special case of a linear system.) That the system does remain linear after quantization has been demonstrated in [14].

In the presence of a potential the Hamiltonian becomes²

$$H = \sqrt{\left(\frac{J - \bar{J}}{2i}\right)^2 - p^3 V(\phi)}, \quad (22)$$

²As written, this refers to exponentials depending only on connection components while recent investigations of loop quantum cosmology have suggested the use of triad dependent holonomies, i.e. $\alpha(p)$ in $e^{i\alpha c}$, in Hamiltonian constraint operators [12, 22, 23]. While basic holonomies in the holonomy-flux algebra do not depend on triad components, the appearance of triad dependent holonomies can be motivated by lattice refinements of an inhomogeneous state occurring in a physical state. Our following discussion of the qualitative behavior does not depend much on which form of holonomies is used in the constraint since alternative cases can be mapped into each other by canonical transformations of (p, J) before quantization.

which we again treat perturbatively. The expansion in V reads

$$H = \frac{J - \bar{J}}{2i} - i \frac{p^3}{J - \bar{J}} V(\phi) + O(V^2(\phi)). \quad (23)$$

After quantization, we again obtain an equation of the form (19). In the variables used here, (p, J) , we can use loop techniques and quantize J using holonomies. If we choose the ordering $\hat{J} = \widehat{\hat{p}e^{ic}}$, basic commutators are

$$[\hat{p}, \hat{J}] = \hbar \hat{J} \quad , \quad [\hat{p}, \hat{J}^\dagger] = -\hbar \hat{J}^\dagger \quad , \quad [\hat{J}, \hat{J}^\dagger] = -2\hbar(p + \hbar/2). \quad (24)$$

Quantum Poisson brackets obtained by taking expectation values of these equations are thus corrected compared to the classical ones:

$$\{p, J\} = -iJ \quad , \quad \{p, \bar{J}\} = i\bar{J} \quad , \quad \{J, \bar{J}\} = 2i(p + \hbar/2). \quad (25)$$

Moreover, in these variables there are more than three fluctuation parameters, namely G^{pp} , $G^{J\bar{J}}$, G^{pJ} , $G^{p\bar{J}}$, G^{JJ} and $G^{\bar{J}\bar{J}}$, since we are using one complex variable J . These quantum variables are defined analogously as with canonical variables, e.g.

$$G^{J\bar{J}} = \frac{1}{2} \langle \hat{J} \hat{J}^\dagger + \hat{J}^\dagger \hat{J} \rangle - J \bar{J}.$$

They are restricted to the correct number by reality conditions $G^{p\bar{J}} = \overline{G^{pJ}}$, $G^{\bar{J}\bar{J}} = \overline{G^{JJ}}$ as well as

$$|J|^2 - (p + \frac{1}{2}\hbar)^2 = G^{pp} - G^{J\bar{J}} + \frac{1}{4}\hbar^2 = \frac{1}{4}\hbar^2 - c_1. \quad (26)$$

as a consequence of $\hat{J}\hat{J}^\dagger = \hat{p}^2$. ($G^{J\bar{J}} - G^{pp} =: c_1$ turns out to be a constant of motion for the free model. Due to its appearance in the reality condition it plays an important role which will also be seen in the perturbed models discussed in what follows.)

Dynamically, the difference to the Wheeler–DeWitt case is that \hat{H} in a metric or triad representation is a difference rather than differential operator [24, 20]. Instead of a partial differential equation in the presence of a scalar we then have a partial difference-differential equation (see also [25, 26]). This is recognizable in our treatment only indirectly since we only implicitly deal with constraint equations for states. We rather express the information contained in the equation for a state through equations implied for expectation values, fluctuations and, if needed, higher moments of the state. The main effect then is the presence of J or e^{ic} , not c itself, in equations of motion. Also effective equations will then initially depend on e^{ic} instead of c , which suggests that they are simply obtained by a replacement of c by $\sin c$ as the real quantity having c as the low curvature limit for $c \ll 1$. However, this replacement on its own overlooks coupling terms of fluctuations which will be analyzed in this paper to provide a complete set of effective equations.

The replacement of c by $\sin c$ is complete for the free model as shown in [14] and indicated by the numerical studies of [10, 11]. In this case, the quantum Hamiltonian lacks

coupling terms from fluctuations and free solutions

$$p_{V=0}(\phi) = \frac{1}{2}(Ae^{-\phi} + Be^{\phi}) - \frac{1}{2}\hbar \quad (27)$$

$$J_{V=0}(\phi) = \frac{1}{2}(Ae^{-\phi} - Be^{\phi}) + iH_0 \quad (28)$$

for expectation values and

$$G_{V=0}^{pp}(\phi) = \frac{1}{2}(c_3e^{-2\phi} + c_4e^{2\phi}) - \frac{1}{4}(c_1 + c_3) \quad (29)$$

$$G_{V=0}^{JJ}(\phi) = \frac{1}{2}(c_3e^{-2\phi} + c_4e^{2\phi}) + \frac{1}{2}(3c_2 - c_1) - 2i(c_5e^{\phi} - c_6e^{-\phi}) = \overline{G_{V=0}^{J\bar{J}}}(\phi) \quad (30)$$

$$G_{V=0}^{pJ}(\phi) = \frac{1}{2}(c_3e^{-2\phi} - c_4e^{2\phi}) + i(c_5e^{\phi} + c_6e^{-\phi}) = \overline{G_{V=0}^{p\bar{J}}}(\phi) \quad (31)$$

$$G_{V=0}^{J\bar{J}}(\phi) = \frac{1}{2}(c_3e^{-2\phi} + c_4e^{2\phi}) + \frac{1}{4}(3c_1 - c_2). \quad (32)$$

for all fluctuations can be determined explicitly.

3 Effective equations

Hamiltonian operators determine the evolution equation (19) for a wave function ψ . Equivalently, a state can be described in terms of its moments, or its expectation values of basic operators together with quantum variables. As already used in (10) and seen in detail later, a Hamiltonian operator can then also be used to derive equations of motion for these infinitely many variables directly, without taking the detour of a wave function. These infinitely many equations are in general coupled and difficult to analyze. Effective equations provide a well-defined scheme to control these equations by formulating them as equations of motion for the classical variables c and p identified with expectation values, or for a larger but finite set including also some of the quantum variables. Such equations can be obtained by systematic approximations (mainly the semiclassical one) to neglect most of the moments, or by solving for all but finitely many of the quantum variables *in terms of those variables to be retained* and inserting those solutions into the equations of motion for the variables to be retained. In the simplest case, one thus obtains effective equations for c and p amended by terms such as an effective potential depending on c and p . This is different from other methods such as perturbation schemes where solutions are already obtained as functions of time; one would solve all the equations up to a certain order but *including those for c and p* to find solutions. Solving for or eliminating only quantum variables but keeping a finite set of variables free requires different techniques. The result of such a procedure, a set of effective equations, will be much more powerful than perturbative solutions since it will illustrate quantum effects more directly and more generally by equations of motion (e.g. containing an effective potential) rather than only through specific solutions.

In general, the derivation of effective equations is more complicated than perturbative solution procedures, and it is not even guaranteed that effective equations of a given type exist to describe a certain regime of interest well. The key step in their derivation is a decoupling of the infinitely many equations for moments of a quantum system such that almost all of them can be solved at least approximately (or shown to be negligible) in terms of a finite set of remaining variables. The main tool to achieve this is often an adiabatic expansion for quantum variables which, for instance, provides the low energy effective action for anharmonic oscillators in quantum mechanics. But quantum variables such as fluctuations need not behave adiabatically in a given regime, or only certain combinations may behave so. Thus, in general the procedure of effective equations is not guaranteed to be of success. As we will see now, quantum cosmology provides examples for regimes where effective equations of adiabatic type do not exist. Nevertheless, as we will also show, bounces in loop quantum cosmology can, fortunately, be described by effective equations even though they turn out to be rather involved.

3.1 Effective equations in quantum cosmology

As shown in [14, 15] and recalled in the preceding section, for a specific ordering of Hamiltonian constraint operators the equations of motion (10) for expectation values of the triad p and connection c describing an isotropic universe sourced by a free, massless scalar do not depend on any quantum variables. They can not only be taken immediately as effective equations without genuine quantum corrections but even describe the system exactly. This is analogous to the equations governing expectation values of a harmonic oscillator or free field theory state. It is true not only in the Wheeler–DeWitt quantization but even in a loop quantization of the same model in appropriate variables. The replacement of connection components c by “holonomies” $\sin c$ in the constraint and the Friedmann equation, as often done as a shortcut to loop effective equations, is thus strictly justified for these models. In the presence of a potential, however, the situation is more complicated and additional quantum corrections arise from the back-reaction of fluctuations on the behavior of expectation values. These corrections can be crucial and must be determined for a robust analysis of quantum systems. This is analogous to adding an anharmonic contribution to the harmonic oscillator, or interaction terms to a free quantum field theory.

In the latter, well-known cases an adiabatic approximation can be employed usefully to describe the quantum behavior around the ground or vacuum state of the system. Some of these corrections take into account properties of the *interacting vacuum state* as opposed to the free vacuum, or of *dynamical coherent states* as opposed to just kinematical ones. Quantum corrections can be computed order by order in an expansion in \hbar combined with the adiabatic one. While the \hbar -expansion is always of interest to capture quantum effects in semiclassical regimes, an adiabatic expansion has to be justified independently. For perturbations around ground states of the harmonic oscillator or free field theories this is clearly reasonable: The exact states (simple Gaussians) of the unperturbed theories have constant fluctuations, and thus perturbations should result only in a weak time dependence. This expectation is borne out self-consistently by the fact that the adiabatic approximation

even with interaction terms provides well-defined solutions.

The situation is different, however, for the quantum cosmological models studied here. We do have a solvable system which can provide the zeroth order for such an expansion, but it lacks a ground state or an otherwise distinguished state in which fluctuations and other quantum variables would be constant. Instead, exact solutions (12)–(16) for the Wheeler–DeWitt model and (27)–(32) for the loop quantization in the absence of interactions show that most quantum variables are exponential functions of time. It is thus not clear a priori which combination of quantum variables, if any, can be treated adiabatically. Nevertheless, any candidate can be analyzed self-consistently by trying to set up an adiabatic approximation. As we will see in the descriptions that follow, several subtleties arise in this process. It clearly demonstrates that for general systems in loop quantum cosmology there is much more to an effective analysis than a simple replacement of connection components c by $\sin c$. We will discuss this issue further in our Conclusions section, after providing a detailed analysis of effective descriptions.

3.2 The Wheeler–DeWitt model

We start with an attempt to develop effective equations based on an adiabaticity assumption for quantum variables. While this will ultimately be unsuccessful, it illustrates the main procedure and several difficulties which can arise. After that we describe possible choices of other combinations of the variables which may be assumed to be adiabatic, although none of them will result in well-defined effective equations for the Wheeler–DeWitt model. In view of a comparison with the loop model, and to confirm that the analyzed cases do not lead to consistent effective equations, it is nevertheless instructive to go through some of the details. In the next section, we will study a different, higher-dimensional type of effective equations which does exist.

To derive effective equations from a Hamiltonian operator \hat{H} one first writes the expectation value of \hat{H} in a general state as a functional of expectation values, spreads and higher moments, captured in quantum variables

$$G^{a,n} = \langle ((\hat{c} - \langle \hat{c} \rangle)^{n-a} (\hat{p} - \langle \hat{p} \rangle)^a)_{\text{Weyl}} \rangle \quad (33)$$

for $2 \leq n \in \mathbb{Z}$ and $0 \leq a \leq n$. This is possible because, with certain restrictions such as uncertainty relations discussed below, the quantum variables together with expectation values allow one to reconstruct the state $\psi(c, p, G^{a,n})$ which has been used in computing the expectation value of \hat{H} . Thus, the quantum Hamiltonian $H_Q(c, p, G^{a,n}) = \langle \psi(c, p, G^{a,n}) | \hat{H} | \psi(c, p, G^{a,n}) \rangle$ is a function of expectation values c and p and quantum variables $G^{a,n}$. Due to the square root present in H it is difficult to write an explicit Hamiltonian operator in our case. Fortunately, this can be circumvented in our framework where we do not work with states and operators directly but with the coupled dynamics of expectation values and quantum variables. We thus implicitly define a Hamiltonian operator, order by order in a perturbation expansion as follows.

The quantum Hamiltonian can be obtained by formally expanding

$$\begin{aligned} H_Q = \langle H(\hat{c}, \hat{p}) \rangle &= \langle H(c + (\hat{c} - c), p + (\hat{p} - p)) \rangle \\ &= \sum_{n=0}^{\infty} \sum_{a=0}^n \frac{1}{n!} \binom{n}{a} \frac{\partial^n H(c, p)}{\partial p^a \partial c^{n-a}} G^{a,n} \end{aligned} \quad (34)$$

in $\hat{c} - c$ and $\hat{p} - p$ (with $G^{a,1}$ understood as taking the value one, i.e. we use normalization of states; for $n = 1$ we have $G^{a,1} = 0$ by definition). Higher order terms in these expansion parameters then combine to correction terms to the classical Hamiltonian containing quantum variables:

$$H_Q = cp - \frac{1}{2} \frac{p^2}{c} V(\phi) - \frac{p^2}{2c^3} V(\phi) G^{cc} + \left(1 + \frac{p}{c^2} V(\phi)\right) G^{cp} - \frac{1}{2c} V(\phi) G^{pp} + \dots \quad (35)$$

where we restrict ourselves to positive p from now on. Since we treat ϕ as an internal time variable, we do not include quantum variables of ϕ and p_ϕ or any correlations between matter and metric degrees of freedom. We do, however, include fluctuations and correlations of the gravitational variables relevant to the given orders, which is second in moments and first in the potential. Note that this suggests correction terms in an effective potential of the form

$$V_{\text{eff}}(\phi) = (1 + c^{-2} G^{cc}(\phi) - 2c^{-1} p^{-1} G^{cp}(\phi) + p^{-2} G^{pp}(\phi)) V(\phi) \sim (1 + C_3 - 2C_4 + C_5) V(\phi) \quad (36)$$

(if we use the free solutions in the second step) and a “zero point energy” $G^{cp} \sim C_4$, which is independent of the expectation values, to the Hamiltonian. To use this for an effective Hamiltonian in terms of c and p only, we would have to solve consistently for the quantum variables by appropriate means. A precise realization, as we will see, turns out to be more complicated.

Equations of motion for expectation values and quantum variables are derived from quantum commutators determining Poisson brackets between expectation values and all the quantum variables. For instance, we have $\{c, p\} = \langle [\hat{c}, \hat{p}] \rangle / i\hbar = 1$ and, using the Leibniz rule,

$$\{G^{pp}, G^{cp}\} = \{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2, \frac{1}{2} \langle \hat{c} \hat{p} + \hat{p} \hat{c} \rangle - \langle \hat{c} \rangle \langle \hat{p} \rangle\} = -2G^{pp} \quad (37)$$

$$\{G^{cc}, G^{cp}\} = 2G^{cc} \quad (38)$$

$$\{G^{cc}, G^{pp}\} = 4G^{cp}. \quad (39)$$

General formulas are provided in [16]. Equations of motion on this infinite dimensional phase space derived from the quantum Hamiltonian $H_Q(c, p, G^{a,n}) = \langle \hat{H} \rangle$ agree with the quantum evolution equations determined from commutators with the Hamiltonian operator. From the quantum Hamiltonian (35) we then obtain equations of motion

$$\begin{aligned} \dot{c} &= \{c, H_Q\} = p - \frac{p}{c} \left(1 + c^{-2} G^{cc} - (cp)^{-1} G^{cp}\right) V(\phi), \\ \dot{p} &= \{p, H_Q\} = -c - \frac{1}{2} \frac{p^2}{c^2} \left(1 + \frac{3}{2} c^{-2} G^{cc} - 4(cp)^{-1} G^{cp} + \frac{1}{2} p^{-2} G^{pp}\right) V(\phi), \end{aligned} \quad (40)$$

$$\dot{G}^{a,2} = \{G^{a,2}, H_Q\} = a \frac{p^2}{c^3} V(\phi) G^{a-1,2} + 2(1-a) \left(1 + \frac{p}{c^2} V(\phi)\right) G^{a,2} - (2-a) \frac{1}{c} V(\phi) G^{a+1,2}.$$

3.2.1 Non-adiabaticity of quantum variables

To analyze possible adiabaticity of fluctuations, we use their equations of motion

$$\dot{G}^{cc} = 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G_0^{cc} - \frac{2}{c} V(\phi) G_0^{cp}, \quad (41)$$

$$\dot{G}^{cp} = \frac{p^2}{c^3} V(\phi) G_0^{cc} - \frac{1}{c} V(\phi) G_0^{pp}, \quad (42)$$

$$\dot{G}^{pp} = 2 \frac{p^2}{c^3} V(\phi) G_0^{cp} - 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G_0^{pp}. \quad (43)$$

These will be the only equations needed for the order we are interested in. An adiabatic approximation proceeds by expanding the fluctuations as $G^{a,2} = \sum_{e=0}^{\infty} \lambda^e G_e^{a,2}$, replacing $d/d\phi$ by $\lambda d/d\phi$ in the equations of motion and expanding the resulting equations in λ . One can then solve order by order for $G_e^{a,2}$ and sum the contributions. The adiabatic approximation to a given order N is the sum $G_N^{a,2} = (\sum_{e=0}^N \lambda^e G_e^{a,2})|_{\lambda=1}$. As the example of the low energy effective action for anharmonic oscillators shows, the zeroth order is already sufficient to derive an effective potential, and quantum corrections to the mass will be obtained at second order [16, 17].

Proceeding in this way, we obtain equations

$$0 = 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G_0^{cc} - \frac{2}{c} V(\phi) G_0^{cp}, \quad (44)$$

$$0 = \frac{p^2}{c^3} V(\phi) G_0^{cc} - \frac{1}{c} V(\phi) G_0^{pp}, \quad (45)$$

$$0 = 2 \frac{p^2}{c^3} V(\phi) G_0^{cp} - 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G_0^{pp} \quad (46)$$

solved by

$$G_0^{cp} = \frac{c}{V(\phi)} \left(1 + \frac{p}{c^2} V(\phi) \right) G_0^{cc}, \quad (47)$$

$$G_0^{pp} = \frac{p^2}{c^2} G_0^{cc} \quad (48)$$

in terms of G_0^{cc} . Only these two relations follow since (44)–(46) presents a degenerate system of linear equations. This is a general property in these variables since the equations are derived with the degenerate Poisson algebra (37)–(39) of three fluctuation variables. The free variable G_0^{cc} , which in general can be a function on phase space and of ϕ , has to be determined at least up to a finite number of constants which specify the state used to expand around. Such a restriction arises by considering the next order: At first adiabatic order we have equations

$$\dot{G}_0^{cc} = 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G_1^{cc} - \frac{2}{c} V(\phi) G_1^{cp}, \quad (49)$$

$$\dot{G}_0^{cp} = \frac{p^2}{c^3} V(\phi) G_1^{cc} - \frac{1}{c} V(\phi) G_1^{pp}, \quad (50)$$

$$\dot{G}_0^{pp} = 2 \frac{p^2}{c^3} V(\phi) G_1^{cp} - 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G_1^{pp} \quad (51)$$

which is again a degenerate linear system, but now an inhomogeneous one for $G_1^{a,2}$. This can only be solved for the $G_1^{a,2}$ provided that the relation

$$\begin{aligned} 0 &= \frac{p^2}{c^2} \dot{G}_0^{cc} + \dot{G}_0^{pp} - 2 \frac{c}{V(\phi)} \left(1 + \frac{p}{c^2} V(\phi) \right) \dot{G}_0^{cp} \\ &= \frac{p^2}{c^2} \dot{G}_0^{cc} + \frac{d}{d\phi} \left(\frac{p^2}{c^2} G_0^{cc} \right) - 2 \left(\frac{p}{c} + \frac{c}{V(\phi)} \right) \frac{d}{d\phi} \left(\left(\frac{p}{c} + \frac{c}{V(\phi)} \right) G_0^{cc} \right) \end{aligned} \quad (52)$$

is satisfied, a differential equation which in fact determines G_0^{cc} up to a constant. One can solve this equation for arbitrary potential $V(\phi)$ by

$$G_0^{cc} = \frac{xV(\phi)}{\sqrt{c^2 + 2pV(\phi)}} \quad (53)$$

with the constant of integration x , and thus

$$G_0^{cp} = \frac{xc(1 + pV(\phi)/c^2)}{\sqrt{c^2 + 2pV(\phi)}}, \quad (54)$$

$$G_0^{pp} = \frac{xp^2V(\phi)/c^2}{\sqrt{c^2 + 2pV(\phi)}}. \quad (55)$$

Note that the initially worrisome inverse $V(\phi)$ in (47) drops out of the final expressions which are perturbative in $V(\phi)$. Nevertheless, having to divide by the potential in an intermediate step will turn out to be problematic. This feature will be cured in the loop quantized model.

These solutions can now be inserted into the equations of motion for c and p to obtain candidate effective equations to zeroth adiabatic order

$$\begin{aligned} \dot{c} &= c - \frac{p}{c} \left(1 - \frac{x}{p\sqrt{c^2 + 2pV(\phi)}} \right) V(\phi) \\ &\sim c - \frac{p}{c} \left(1 - \frac{x}{cp} + \frac{x}{c^3} V(\phi) \right) V(\phi) + O((pV/c^2)^3) \end{aligned} \quad (56)$$

$$\begin{aligned} \dot{p} &= -p + -\frac{p^2}{2c^2} \left(1 - \frac{4x}{p\sqrt{c^2 + 2pV(\phi)}} \right) V(\phi) \\ &\sim -p - \frac{p^2}{2c^2} \left(1 - \frac{4x}{cp} + \frac{4x}{c^3} V(\phi) \right) V(\phi) + O((pV/c^2)^3) \end{aligned} \quad (57)$$

There is no \hbar in these effective equations, but the free variable x parameterizes fluctuations of a state. It should thus be expected to be of the order \hbar for effective equations corresponding to states saturating the uncertainty relation

$$G^{cc}G^{pp} - (G^{cp})^2 \geq \frac{\hbar^2}{4}. \quad (58)$$

However, when trying to implement these relations, we recognize that the effective equations are inconsistent because there is in fact no state corresponding to this evolution: uncertainty relations are not satisfied. Inserting our solutions to zeroth order in the adiabatic expansion, we obtain

$$G_0^{cc}G_0^{pp} - (G_0^{cp})^2 = -\frac{c^2}{V(\phi)^2} \left(1 + 2\frac{pV(\phi)}{c^2}\right) (G_0^{cc})^2 < 0$$

for $pV \ll c^2$. Thus, there is no choice for the only free parameter x in G_0^{cc} which would make the adiabatic solution consistent with the uncertainty relation. This illustrates how one can self-consistently test whether an assumption of adiabaticity for certain variables results in reliable effective equations. Although the adiabaticity assumption for quantum variables has not resulted in consistent effective equations, Eqs. (56) and (57) suggest that true effective equations are more involved than just implying an effective potential (36): There are new expectation value dependent coefficients, and higher powers of the classical potential. In what follows we will look at other adiabaticity assumptions, before turning to higher dimensional effective equations in the next section.

3.2.2 Non-perturbative potential

Before changing our adiabaticity assumption, we probe whether the perturbative treatment of the potential may be responsible for the non-existence of effective equations. There could, after all, be regimes in which the potential is important in making quantum variables adiabatic. We thus start from a non-expanded classical Hamiltonian $H = p\sqrt{c^2 - pV(\phi)}$ and obtain the quantum Hamiltonian

$$\begin{aligned} H_Q = & p\sqrt{c^2 - pV(\phi)} - \frac{p^2V(\phi)}{2(c^2 - pV(\phi))^{3/2}}G^{cc} + \frac{c^3 - cpV(\phi)/2}{(c^2 - pV(\phi))^{3/2}}G^{cp} \\ & - \frac{c^2 - 3pV(\phi)/4}{2(c^2 - pV(\phi))^{3/2}}V(\phi)G^{pp} + \dots \end{aligned} \quad (59)$$

up to second order in quantum variables. Now, the zeroth order adiabatic solutions take the form

$$G_0^{cp} = \frac{c}{V(\phi)} \frac{c^2 - pV(\phi)/2}{c^2 - 3pV(\phi)/4} G_0^{cc} \quad (60)$$

$$G_0^{pp} = \frac{p^2}{c^2 - 3pV(\phi)/4} G_0^{cc} \quad (61)$$

and the uncertainty product

$$G_0^{cc}G_0^{pp} - (G_0^{cp})^2 = -\frac{c^2}{V(\phi)^2} \frac{1 - \frac{p}{c^2}V(\phi) - \frac{3}{4}\left(\frac{p}{c^2}V(\phi)\right)^2 + \frac{3}{4}\left(\frac{p}{c^2}V(\phi)\right)^3}{\left(1 - \frac{3}{4}\frac{p}{c^2}V(\phi)\right)} (G_0^{cc})^2$$

is still negative independently of the potential in the allowed range $|pV(\phi)|/c^2 < 1$. (Allowing larger potentials would give only a narrow range $1 < pV(\phi)/c^2 < 2/\sqrt{3} \approx 1.155$ where

the previous expression would be positive. But then no real p_ϕ is possible. Thus, dropping the assumption of a perturbative potential does not, by itself, give rise to consistent effective equations.

3.2.3 Non-adiabaticity relative to expectation values

While none of the quantum variables in (12)–(16) is constant for a given state of the free Wheeler–DeWitt model which one may choose to perturb around, relative fluctuations G^{cc}/c^2 and G^{pp}/p^2 are constant, and similarly for other quantum variables. One may thus try an adiabatic approximation for those combinations rather than one directly in terms of quantum variables which fails, as we saw. Let us now assume that variables of the form

$$g^{a,n} := c^{-n+a+l} p^{-a+l} G^{a,n} \quad (62)$$

behave adiabatically where l is some fixed integer to be chosen. For the free solutions, the $g^{a,n}$ will be constant for any l since cp is constant, and thus adiabaticity seems more likely. (The constants C_I in the free solutions are not necessary to keep in the definition of $g^{a,n}$ since they can be absorbed without changing adiabaticity properties.)

Equations of motion for the new variables follow from the product rule:

$$\begin{aligned} \dot{g}^{cc} &= \frac{pV(\phi)}{c(c^2 - pV(\phi))^{3/2}} \left(\frac{3}{2} ((l + 8/3)c^2 - (l + 2)pV(\phi)) g^{cc} - 2(c^2 - 3pV(\phi)/4) g^{cp} \right), \\ \dot{g}^{cp} &= \frac{pV(\phi)}{c(c^2 - pV(\phi))^{3/2}} \left(c^2 g^{cc} + \frac{3}{2}(l + 1)(c^2 - pV(\phi)) g^{cp} - (c^2 - 3pV(\phi)/4) g^{pp} \right), \\ \dot{g}^{pp} &= \frac{pV(\phi)}{c(c^2 - pV(\phi))^{3/2}} \left(2c^2 g^{cp} + \frac{3}{2} ((l - 3/2)c^2 - lpV(\phi)) g^{pp} \right) \end{aligned}$$

where we ignore quadratic terms in $g^{a,n}$. The zeroth order adiabatic solutions are

$$g_0^{cp} = \frac{3(l + 8/3)c^2 - (l + 2)pV(\phi)}{4(c^2 - 3pV(\phi)/4)} g_0^{cc}, \quad (63)$$

$$g_0^{pp} = -\frac{c^2((l + 8/3)c^2 - (l + 2)pV(\phi))}{(c^2 - 3pV(\phi)/4)((l - 2/3)c^2 - lpV(\phi))} g_0^{cc} \quad (64)$$

which solves the remaining zeroth order equation only for $l = 0$, $l = 1$ or $l = 2$.

The case $l = 0$, i.e. an assumption of adiabaticity for $g^{cc} = G^{cc}/c^2$, $g^{cp} = G^{cp}/cp$ and $g^{pp} = G^{pp}/p^2$, gives solutions $g_0^{cp} = 2g_0^{cc}$ and $g_0^{pp} = 4g_0^{cc}$ which in this case are actually exact to any adiabatic order. However, the uncertainty product $c^2 p^2 g^{cc} g^{pp} - (cp g^{cp})^2$ now vanishes for any choice of free parameters and uncertainty relations are still violated. This happens only marginally since for a slightly positive value one could choose the free parameter, analogous to x before, large enough to ensure that the uncertainty relation is satisfied. It could happen that higher orders of the adiabatic expansion would make the uncertainty product positive, but we do not pursue this here since, if successful, it would most likely give only special regimes where effective equations would be valid.

For $l = 1$ we obtain

$$g_0^{cp} = \frac{\frac{5}{2}c^2 - \frac{3}{2}pV(\phi)}{2(c^2 - \frac{3}{4}pV(\phi))}g_0^{cc} \quad \text{and} \quad g_0^{pp} = \frac{c^2}{c^2 - \frac{3}{4}pV(\phi)}g_0^{cc}$$

with a negative uncertainty product. For $l = 2$, we have

$$g_0^{cp} = \frac{c^2}{2(c^2 - \frac{3}{4}pV(\phi))}g_0^{cc} \quad \text{and} \quad g_0^{pp} = \frac{c^4}{4(c^2 - \frac{3}{4}pV(\phi))^2}g_0^{cc}$$

with a vanishing uncertainty product. None of these cases gives a consistent set of effective equations.

3.2.4 Additive non-adiabaticity

Instead of factorizing off the time dependence of the free solutions as in the variables $g^{a,n}$, one can try to subtract it off, i.e. attempt an adiabatic expansion in $G^{cc} - C_3c^2$, $G^{cp} - C_4cp$ and $G^{pp} - C_5p^2$. In contrast to the previous case the equations now also depend on parameters C_I of the free solutions. It is easy to derive the resulting equations which, at any adiabatic order, provides a set of inhomogeneous linear equations for the quantum variables. There are three equations for three fluctuation parameters, but with a vanishing determinant of the linear system. It turns out that the inhomogeneity resulting from subtracting off the zeroth order solutions does not allow any solution. Thus, also adiabaticity additive to the zeroth order solutions is not realized.

3.2.5 Non-adiabaticity with respect to free solutions

Had one of the previous attempts succeeded in providing effective equations, the result would have been time dependent only through the scalar potential $V(\phi)$ as is clear from the examples provided. Our final attempt brings in even stronger time dependence by assuming again adiabaticity relative to free solutions, but using the free solutions (12)–(16) in explicit, time dependent form $G_{V=0}^{a,n}(\phi)$ rather than implicitly as, e.g., $G_{V=0}^{cc} \propto c^2$ before. Thus, we now assume that variables $g^{a,n} := G^{a,n}/G_{V=0}^{a,n}(\phi)$ are adiabatic. The new variables satisfy equations of motion

$$\dot{g}^{a,n} = \frac{\dot{G}^{a,n}}{G_{V=0}^{a,n}(\phi)} - \frac{\dot{G}_{V=0}^{a,n}(\phi)}{G_{V=0}^{a,n}(\phi)}g^{a,n}$$

or explicitly

$$\dot{g}^{cc} = -2 \left(1 - \frac{c(c^2 - pV(\phi)/2)}{(c^2 - pV(\phi))^{3/2}} \right) g^{cc} - 2V(\phi) \frac{c^2 - 3pV(\phi)/4}{(c^2 - pV(\phi))^{3/2}} \frac{G_{V=0}^{cp}(\phi)}{G_{V=0}^{cc}(\phi)} g^{cp}, \quad (65)$$

$$\dot{g}^{cc} = \frac{p^2V(\phi)}{(c^2 - pV(\phi))^{3/2}} \frac{G_{V=0}^{cc}(\phi)}{G_{V=0}^{cp}(\phi)} g^{cc} - V(\phi) \frac{c^2 - 3pV(\phi)/4}{(c^2 - pV(\phi))^{3/2}} \frac{G_{V=0}^{pp}(\phi)}{G_{V=0}^{cp}(\phi)} g^{pp}, \quad (66)$$

$$\dot{g}^{pp} = 2 \frac{p^2V(\phi)}{(c^2 - pV(\phi))^{3/2}} \frac{G_{V=0}^{cp}(\phi)}{G_{V=0}^{pp}(\phi)} g^{cp} + 2 \left(1 - \frac{c(c^2 - pV(\phi)/2)}{(c^2 - pV(\phi))^{3/2}} \right) g^{pp}. \quad (67)$$

To zeroth order, adiabatic solutions would be given by

$$\begin{aligned} g_0^{cp} &= \frac{c(c^2 - pV(\phi)/2) - (c^2 - pV(\phi))^{3/2} \frac{G_{V=0}^{cc}(\phi)}{G_{V=0}^{cp}(\phi)}}{V(\phi)(c^2 - 3pV(\phi)/4)} g_0^{cc}, \\ g_0^{pp} &= \frac{p^2}{c^2 - 3pV(\phi)/4} \frac{G_{V=0}^{cc}(\phi)}{G_{V=0}^{pp}(\phi)} g_0^{cc} \end{aligned}$$

which, when inserted into equations of motion for c and p would give time dependent terms not only through $V(\phi)$ but also through $G_{V=0}^{a,2}(\phi)$. This is an exponential time dependence and thus stronger than that of a polynomial potential $V(\phi)$. However, also here the result is not consistent since the uncertainty product

$$G_{V=0}^{cc}(\phi)g^{cc}G_{V=0}^{pp}(\phi)g^{pp} - (G_{V=0}^{cp}(\phi)g^{cp})^2 \sim -\frac{p^4V(\phi)^2}{64c^2(c^2 - 3pV(\phi)/4)^2}(G_{V=0}^{cc}(\phi))^2(g_0^{cc})^2$$

to leading order in $pV(\phi)/c^2$ is again negative.

We did not manage to find a choice of adiabatic variables which would give rise to consistent effective equations. However, since some cases led only to marginal violations of the uncertainty relation, one may still be hopeful that a choice exists. More importantly, changes to the equations of motion such as those by a loop quantization could possibly lead to the existence of consistent effective equations which we will probe next.

3.3 Effective equations of loop quantum cosmology

The solvable loop model is formulated in non-canonical variables, satisfying a Poisson algebra different from that of the Wheeler–DeWitt model. Thus, also the procedure of deriving effective equations is different and has to be analyzed anew. We must now consider two different sets of quantum variables, each one related to J or \bar{J} . We will first obtain general equations of motion for these variables, which are then to be restricted by reality conditions ensuring that $J\bar{J} = p^2$ or, at the quantum level, $\hat{J}\hat{J}^\dagger = \hat{p}^2$. Expanded in powers of quantum variables, the quantum Hamiltonian reads

$$\begin{aligned} H_Q &= \frac{J - \bar{J}}{2i} - i\frac{p^3V(\phi)}{J - \bar{J}} - i\frac{p^3V(\phi)}{(J - \bar{J})^3} \left(G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}} \right) \\ &\quad + 3i\frac{p^2V(\phi)}{(J - \bar{J})^2} \left(G^{pJ} - G^{p\bar{J}} \right) - 3i\frac{pV(\phi)}{J - \bar{J}} G^{pp} + \dots \end{aligned} \quad (68)$$

From now on we ignore terms of higher moments since they will be subdominant in a semiclassical expansion. Higher moments of typical semiclassical states are smaller at higher orders. Moreover, a moment of order n appears in the quantum Hamiltonian with a coefficient obtained by an n -th derivative of the classical Hamiltonian; see (34). Higher moments of order n are thus suppressed by additional small factors of the form $p^{-k}(J - \bar{J})^{-n+k}$ compared to the classical perturbation term. There is a subtlety with this argument when looking at equations of motion: In Poisson brackets $\{G^{a,n}, G^{b,m}\}$ with $n + m \geq 4$

(formally including $n = 1$ or $m = 1$ as expectation values) there can not only be linear terms of moments of order $n+m-1$, as in the basic relations (69)–(77) below, but also terms of the form $\langle \cdot \rangle^l G^{c,n+m-1-l}$ for $0 \leq l \leq n+m-3$, as illustrated by the examples in App. A. (Also \hbar^k -terms appear, but they play a role only at higher orders.) Depending on the powers l realized, the expectation value dependent prefactors could, in equations of motion, cancel suppressions involved in coefficients of higher moment terms in the Hamiltonian. This is potentially problematic if the highest allowed powers for l do occur. For instance, we have $\{G^{a,2}, G^{b,2}\}$ of the form $\langle \cdot \rangle G^{c,2}$ with a single factor of expectation values, but in a bracket like $\{G^{a,2}, G^{b,3}\}$ there could be terms $\langle \cdot \rangle^2 G^{c,2}$ with up to two factors. Then, the additional suppression of $G^{b,3}$ in the Hamiltonian would be cancelled in equations of motion by the additional factor in Poisson brackets. It would require one to take into account all terms containing $G^{a,n}$ in the quantum Hamiltonian, which would clearly be unmanageable.

Fortunately, this problem does not arise and there is a consistent way to derive a truncation for equations of motion to any given order: For equations of motion for expectation values, Poisson brackets $\{\langle \cdot \rangle, G^{a,n}\}$ only have terms linear in moments $G^{b,n}$ of the same order as used in the bracket, and possibly terms $\langle \cdot \rangle G^{c,n-1}$ with a single factor of an expectation value. (There may also be terms with higher powers of \hbar which we can safely ignore.) The terms with a single factor of expectation values may arise because taking a commutator of, say, \hat{p} with $(\hat{J} - J)^n$ as it is needed for $\{p, G^{J^n}\}$ replaces one factor of $\hat{J} - J$ by just \hat{J} itself. To bring the result into the form of a moment of order n , one has to add J multiplied with a moment of order $n-1$. The only other terms that may arise in such cases are due to reordering, which contributes higher powers of \hbar . (They would be relevant at higher moment orders than considered here.) Taking into account suppression factors in the Hamiltonian, equations of motion for expectation values thus have suppressions of at least $\langle \cdot \rangle^{1-n}$ in higher moment contributions. Being n -dependent, this leads to higher suppression for higher moments and provides a consistent truncation. The same order of truncation can then be extended to quantum variables by requiring that the reality condition (26) is preserved by the truncated equations of motion. This consistent truncation procedure is illustrated below for moments of up to second order.

While all quantum variables commute with expectation values when defined in terms of canonical variables, quantum variables and expectation values do not Poisson commute for non-canonical variables such as p and J . Following the general scheme used before, Poisson bracket relations between the variables are derived as

$$\{G^{JJ}, p\} = 0 = \{G^{pp}, p\} \quad (69)$$

$$\{G^{pJ}, p\} = iG^{pJ} \quad , \quad \{G^{p\bar{J}}, p\} = -iG^{p\bar{J}} \quad (70)$$

$$\{G^{JJ}, p\} = 2iG^{JJ} \quad , \quad \{G^{\bar{J}\bar{J}}, p\} = -2iG^{\bar{J}\bar{J}} \quad (71)$$

and

$$\{G^{pp}, J\} = -2iG^{pJ} \quad , \quad \{G^{pp}, \bar{J}\} = 2iG^{p\bar{J}}, \quad (72)$$

$$\{G^{J\bar{J}}, J\} = -2iG^{pJ} \quad , \quad \{G^{J\bar{J}}, \bar{J}\} = 2iG^{p\bar{J}}, \quad (73)$$

$$\{G^{pJ}, J\} = -iG^{JJ} \quad , \quad \{G^{pJ}, \bar{J}\} = iG^{J\bar{J}} + 2iG^{pp}, \quad (74)$$

$$\{G^{p\bar{J}}, J\} = -iG^{J\bar{J}} - 2iG^{pp} \quad , \quad \{G^{p\bar{J}}, \bar{J}\} = iG^{J\bar{J}}, \quad (75)$$

$$\{G^{JJ}, J\} = 0 \quad , \quad \{G^{JJ}, \bar{J}\} = 4iG^{pJ}, \quad (76)$$

$$\{G^{J\bar{J}}, J\} = -4iG^{p\bar{J}} \quad , \quad \{G^{J\bar{J}}, \bar{J}\} = 0 \quad (77)$$

between quantum variables and expectation values. Notice that (69), (72) and (73) imply that the difference $G^{J\bar{J}} - G^{pp}$ commutes with any function of p , J and \bar{J} only.

Also in contrast to the Wheeler–DeWitt model whose canonical variables gave rise to a closed Poisson algebra for the fluctuations $G^{a,2}$, Poisson brackets between fluctuations in the loop model involve higher moments due to the non-canonical form of the basic variables (p, J) . Poisson brackets between two fluctuations thus in general depend on a quantum variable of order three, but they also involve fluctuation dependent terms. While the third order variables can be cut off in a semiclassical treatment to the order we are interested in, the latter terms, as we will see below, have to be included in a consistent set of effective equations. We thus need to determine the full set of Poisson brackets between quantum variables of order two. As derived in Appendix A, they are

$$\{G^{pp}, G^{J\bar{J}}\} = -2i(JG^{p\bar{J}} - \bar{J}G^{pJ}) \quad (78)$$

$$\{G^{pp}, G^{JJ}\} = -4iG^{pJJ} - 4iJG^{pJ} = \overline{\{G^{pp}, G^{J\bar{J}}\}} \quad (79)$$

$$\{G^{pp}, G^{pJ}\} = -2iG^{ppJ} - 2iJG^{pp} + \frac{1}{6}i\hbar^2 J = \overline{\{G^{pp}, G^{p\bar{J}}\}} \quad (80)$$

$$\{G^{J\bar{J}}, G^{JJ}\} = -4iG^{pJJ} - 4i(p + \hbar/2)G^{JJ} = \overline{\{G^{J\bar{J}}, G^{J\bar{J}}\}} \quad (81)$$

$$\{G^{J\bar{J}}, G^{pJ}\} = -2iG^{ppJ} - 2i(p + \hbar/2)G^{pJ} + iJG^{J\bar{J}} - i\bar{J}G^{JJ} + \frac{1}{6}i\hbar^2 J = \overline{\{G^{J\bar{J}}, G^{p\bar{J}}\}} \quad (82)$$

$$\{G^{JJ}, G^{pJ}\} = 2iG^{JJJ} + 2iJG^{JJ} = \overline{\{G^{J\bar{J}}, G^{p\bar{J}}\}} \quad (83)$$

$$\{G^{JJ}, G^{p\bar{J}}\} = 6iG^{ppJ} + 8i(p + \hbar/2)G^{pJ} - 2i\bar{J}G^{JJ} - i\hbar^2 J = \overline{\{G^{J\bar{J}}, G^{pJ}\}} \quad (84)$$

$$\begin{aligned} \{G^{JJ}, G^{J\bar{J}}\} &= 8iG^{ppp} + 16i(p + \hbar/2)G^{pp} + 8i(p + \hbar/2)G^{J\bar{J}} - 8iJG^{p\bar{J}} - 8i\bar{J}G^{pJ} \\ &\quad + 4i\hbar^2 p + 2i\hbar^3 \end{aligned} \quad (85)$$

$$\{G^{pJ}, G^{p\bar{J}}\} = 4iG^{ppp} + 6i(p + \hbar/2)G^{pp} - iJG^{p\bar{J}} - i\bar{J}G^{pJ} + \frac{1}{2}i\hbar^2 p + \frac{1}{4}i\hbar^3. \quad (86)$$

The relevant relations for leading order back-reaction effects in the loop model are brackets of the form $\{G^{a,2}, \langle \cdot \rangle\}$ together with contributions of $\{G^{a,2}, G^{b,2}\}$ from moments up to second order. (The fluctuation independent \hbar^2 -terms can to this order be ignored as well since $G^{a,2}$ are typically of order \hbar near saturation of the uncertainty relation.) Expectation values and second moments thus provide a closed system under taking Poisson brackets in this form, albeit a non-linear one.

3.3.1 Equations of motion

Just as the algebra (37)–(39) of fluctuations in canonical variables is degenerate, being given by a Poisson structure on a 3-dimensional manifold, the relations $\{G^{a,2}, \langle \cdot \rangle\}$ are degenerate in the sense that functions of the fluctuations exist which commute with both expectation values p and J . It is easy to see that, as already noted, one such function is linear, $G^{J\bar{J}} - G^{pp} = c_1$. The second function is quadratic,

$$C := 2(G^{pp})^2 + (G^{J\bar{J}})^2 - 4|G^{p\bar{J}}|^2 + |G^{JJ}|^2. \quad (87)$$

(Its value is $C = \frac{3}{4}c_1^2 - \frac{1}{2}c_1c_2 + \frac{3}{4}c_2^2 + 4c_3c_4 + 4c_5c_6$ for the free solutions (27)–(32).) The linear function has one immediate implication: It is exactly this combination which appears in the reality condition (26) implied by $\hat{J}\hat{J}^\dagger = \hat{p}^2$ in the loop quantization. In the free model, the combination $c_1 = G^{J\bar{J}} - G^{pp}$ is a constant of motion. Whether or not this remains true when perturbations are included is an interesting question because the form of the reality condition (corresponding to an implementation of the correct physical inner product) is essential for singularity resolution: it picks out exactly the bouncing solutions in the free model (unless the constant of motion c_1 would be negative and $|c_1|$ large, which is never realized for states of the free model being semiclassical at least once). If the form of the reality condition could be shown to be preserved by quantum corrections, there would be no obvious violations of the bounce as one could in general imagine if c_1 would not remain constant and could evolve to large negative values from initial semiclassical states [15]. If, however, $G^{J\bar{J}} - G^{pp}$ does not remain constant when the free model is perturbed, one would have to be more careful with conclusions about the bounce.

Since the difference $G^{J\bar{J}} - G^{pp}$ commutes with any function of the expectation values, its preservation does not depend on the precise form of the classical Hamiltonian. However, for leading quantum corrections we have to consider fluctuation dependent terms in the quantum Hamiltonian (68), which contribute extra terms to the equations of motion of fluctuations. These fluctuation dependent terms do not necessarily commute with $G^{J\bar{J}} - G^{pp}$.

Using the Poisson relations, we obtain

$$\begin{aligned} \dot{p} = & -\frac{J + \bar{J}}{2} + \frac{J + \bar{J}}{(J - \bar{J})^2} p^3 V(\phi) + 3 \frac{J + \bar{J}}{(J - \bar{J})^4} p^3 (G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}}) V(\phi) \\ & - 6 \frac{J + \bar{J}}{(J - \bar{J})^3} p^2 (G^{pJ} - G^{p\bar{J}}) V(\phi) + 3 \frac{J + \bar{J}}{(J - \bar{J})^2} p G^{pp} V(\phi) \\ & - \frac{2p^3}{(J - \bar{J})^3} (G^{JJ} - G^{\bar{J}\bar{J}}) V(\phi) + \frac{3p^2}{(J - \bar{J})^2} (G^{pJ} + G^{p\bar{J}}) V(\phi) \end{aligned} \quad (88)$$

and

$$\begin{aligned}
\dot{J} = & -(p + \hbar/2) + \left(\frac{3p^2 J}{J - \bar{J}} + \frac{2p^3(p + \hbar/2)}{(J - \bar{J})^2} \right) V(\phi) \\
& + \left(\frac{3p^2 J}{(J - \bar{J})^3} + \frac{6p^3(p + \hbar/2)}{(J - \bar{J})^4} \right) (G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}}) V(\phi) \\
& - 3 \left(\frac{2pJ}{(J - \bar{J})^2} + \frac{4p^2(p + \hbar/2)}{(J - \bar{J})^3} \right) (G^{pJ} - G^{p\bar{J}}) V(\phi) \\
& + 3 \left(\frac{J}{J - \bar{J}} + \frac{2p(p + \hbar/2)}{(J - \bar{J})^2} \right) G^{pp} V(\phi) + 4 \frac{p^3}{(J - \bar{J})^3} (G^{p\bar{J}} - G^{pJ}) V(\phi) \\
& - 3 \frac{p^2}{(J - \bar{J})^2} (G^{JJ} - G^{J\bar{J}} - 2G^{pp}) V(\phi) + 6 \frac{p}{J - \bar{J}} G^{pJ} V(\phi)
\end{aligned} \tag{89}$$

for the expectation values and

$$\begin{aligned}
\dot{G}^{pp} = & - \left(1 - \frac{2p^3}{(J - \bar{J})^2} \right) (G^{pJ} + G^{p\bar{J}}) V(\phi) \\
& - \frac{4p^3}{(J - \bar{J})^3} (JG^{pJ} - \bar{J}G^{p\bar{J}} - JG^{p\bar{J}} + \bar{J}G^{pJ}) V(\phi) \\
& + \frac{6p^2(J + \bar{J})}{(J - \bar{J})^2} G^{pp} V(\phi) - \frac{\hbar^2 p^2 (J + \bar{J})}{2 (J - \bar{J})^2} V(\phi) \\
= & - \left(1 - \frac{2p^3}{(J - \bar{J})^2} \right) (G^{pJ} + G^{p\bar{J}}) V(\phi) - \frac{4p^3(J + \bar{J})}{(J - \bar{J})^3} (G^{pJ} - G^{p\bar{J}}) V(\phi) \\
& + \frac{6p^2(J + \bar{J})}{(J - \bar{J})^2} G^{pp} V(\phi) - \frac{\hbar^2 p^2 (J + \bar{J})}{2 (J - \bar{J})^2} V(\phi)
\end{aligned} \tag{90}$$

and

$$\begin{aligned}
\dot{G}^{J\bar{J}} = & - \left(1 - \frac{2p^3}{(J - \bar{J})^2} \right) (G^{pJ} + G^{p\bar{J}}) V(\phi) - \frac{4p^3(p + \hbar/2)}{(J - \bar{J})^3} (G^{JJ} - G^{\bar{J}\bar{J}}) V(\phi) \\
& - \frac{3p^2}{(J - \bar{J})^2} ((J + \bar{J})G^{J\bar{J}} - (2p + \hbar)(G^{pJ} + G^{p\bar{J}}) - \bar{J}G^{JJ} - JG^{\bar{J}\bar{J}} \\
& + \frac{1}{6}\hbar^2(J + \bar{J})) V(\phi) + \frac{6p}{J - \bar{J}} (JG^{p\bar{J}} - \bar{J}G^{pJ}) V(\phi) \\
= & - \left(1 - 3p - \frac{2p^2(p + 3(p + \hbar/2))}{(J - \bar{J})^2} \right) (G^{pJ} + G^{p\bar{J}}) V(\phi) \\
& - \frac{3p(J + \bar{J})}{J - \bar{J}} (G^{pJ} - G^{p\bar{J}}) V(\phi) - \frac{3}{2} \frac{p^2}{J - \bar{J}} \left(1 + \frac{8}{3} \frac{p(p + \hbar/2)}{(J - \bar{J})^2} \right) (G^{JJ} - G^{\bar{J}\bar{J}}) V(\phi) \\
& + \frac{3}{2} \frac{p^2(J + \bar{J})}{(J - \bar{J})^2} (G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}}) V(\phi) - \frac{\hbar^2 p^2 (J + \bar{J})}{2 (J - \bar{J})^2} V(\phi)
\end{aligned} \tag{91}$$

for the fluctuations featuring in the reality condition, ignoring terms quadratic in fluctuations. A combination gives

$$\begin{aligned}
\dot{G}^{J\bar{J}} - \dot{G}^{pp} &= p \left(3 + \frac{6p(p + \hbar/2)}{(J - \bar{J})^2} \right) (G^{pJ} + G^{p\bar{J}})V(\phi) \\
&\quad + \frac{p(J + \bar{J})}{J - \bar{J}} \left(-3 + 4\frac{p^2}{(J - \bar{J})^2} \right) (G^{pJ} - G^{p\bar{J}})V(\phi) \\
&\quad - \frac{p^2}{J - \bar{J}} \left(\frac{3}{2} + \frac{4p(p + \hbar/2)}{(J - \bar{J})^2} \right) (G^{JJ} - G^{\bar{J}\bar{J}})V(\phi) \\
&\quad + \frac{3p^2(J + \bar{J})}{2(J - \bar{J})^2} (G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}} - 4G^{pp})V(\phi)
\end{aligned} \tag{92}$$

which can be seen to equal $2d(|J|^2 - (p + \hbar/2)^2)/d\phi$ from (88) and (89). Terms included in these equations of motion preserve the reality condition. Thus, this consistent truncation of the quantum equations describes the physical evolution of expectation values and fluctuations as they would be computed from a physical state.

However, these equations also show that the contribution $G^{J\bar{J}} - G^{pp}$ to the reality condition is no longer constant when fluctuation dependent corrections in H_Q are allowed for. It is then possible that the term c_1 , which was constant in the free model and determines whether or not expectation values bounce, changes in time so as to prevent a bounce when small volume is approached during long evolution. A firm conclusion about the presence of a bounce for a massive or interacting scalar thus requires a more detailed analysis taking into account the behavior of fluctuations. We will come back to this issue in the next section.

Equations of motion for the remaining second moments are

$$\begin{aligned}
\dot{G}^{pJ} &= -\frac{1}{2} \left(1 - \frac{2p^3}{(J - \bar{J})^2} \right) (G^{JJ} + G^{J\bar{J}} + 2G^{pp})V(\phi) + \frac{3p^2}{J - \bar{J}} G^{pJ}V(\phi) \\
&\quad + \frac{p^3 V(\phi)}{(J - \bar{J})^3} (-2(J + \bar{J})G^{JJ} - 2JG^{\bar{J}\bar{J}} + 2(p + \hbar/2)(4G^{p\bar{J}} - 2G^{pJ}) + 2JG^{J\bar{J}} \\
&\quad - \hbar^2 \bar{J} + \frac{1}{3}\hbar^2 J) + \frac{3p^2 V(\phi)}{(J - \bar{J})^2} (6(p + \hbar/2)G^{pp} - \bar{J}G^{pJ} - JG^{p\bar{J}} + \frac{1}{2}\hbar^2 p + \frac{1}{4}\hbar^3) \\
&\quad + \frac{3pV(\phi)}{J - \bar{J}} (2JG^{pp} - \frac{1}{6}\hbar^2 J) \\
&= \overline{\dot{G}^{p\bar{J}}}
\end{aligned} \tag{93}$$

and

$$\begin{aligned}
\dot{G}^{JJ} &= -2 \left(1 - \frac{2p^3}{(J - \bar{J})^2} \right) G^{pJ} V(\phi) + \frac{6p^2}{J - \bar{J}} G^{JJ} V(\phi) \\
&\quad + \frac{p^3 V(\phi)}{(J - \bar{J})^3} (8(p + \hbar/2)(2G^{pp} + G^{J\bar{J}} - G^{JJ}) - 8JG^{p\bar{J}} - 8\bar{J}G^{pJ} + 4\hbar^2 p + 2\hbar^3) \\
&\quad - \frac{3p^2 V(\phi)}{(J - \bar{J})^2} (2JG^{JJ} - 8(p + \hbar/2)G^{pJ} + 2\bar{J}G^{JJ} + \hbar^2 J) + \frac{12p}{J - \bar{J}} JG^{pJ} V(\phi) \\
&= \overline{\dot{G}^{J\bar{J}}}.
\end{aligned} \tag{94}$$

As in the Wheeler–DeWitt context, we will now briefly describe attempts to find adiabatic regimes of quantum variables, followed in the next section by a perturbative analysis of the equations of motion.

3.3.2 Non-adiabaticity of quantum variables

For simplicity, we now take into account the classical Hamiltonian as a function of expectation values only in order to compute the leading order terms in equations of motion for fluctuations. These equations are

$$\dot{G}^{pp} = - \left(1 - \frac{2p^3}{(J - \bar{J})^2} V(\phi) \right) (G^{pJ} + G^{p\bar{J}}) = \dot{G}^{J\bar{J}}, \tag{95}$$

$$\dot{G}^{pJ} = -\frac{1}{2} \left(1 - \frac{2p^3}{(J - \bar{J})^2} V(\phi) \right) (G^{JJ} + G^{J\bar{J}} + 2G^{pp}) + \frac{3p^2}{J - \bar{J}} V(\phi) G^{pJ} = \overline{\dot{G}^{p\bar{J}}}, \tag{96}$$

$$\dot{G}^{JJ} = -2 \left(1 - \frac{2p^3}{(J - \bar{J})^2} V(\phi) \right) G^{pJ} + \frac{6p^2}{J - \bar{J}} V(\phi) G^{JJ} = \overline{\dot{G}^{J\bar{J}}}. \tag{97}$$

These are not the complete equations of motion; we use them only to illustrate obstacles to the existence of adiabatic effective equations. The full equations of motion to this order will be used later on for a new type of effective system.

To zeroth order in an adiabatic expansion of the fluctuations, Eq. (95) shows that G_0^{pJ} is purely imaginary, from which Eq. (97) then shows that G_0^{JJ} is real. Moreover, Eq. (97) gives the relation between these two quantities,

$$G_0^{pJ} - G_0^{p\bar{J}} = \frac{3p^2 V(\phi)}{1 - 2p^3 V(\phi)/(J - \bar{J})^2} \frac{G_0^{JJ} + G_0^{J\bar{J}}}{J - \bar{J}} \tag{98}$$

which when used in Eq. (96) leaves only one free function such as G_0^{pp} : to leading order in $p^2 V(\phi)/(J - \bar{J})$ we have

$$G_0^{JJ} + G_0^{J\bar{J}} + 6G_0^{pp} + 2c_1 = \frac{18p^4 V(\phi)^2}{(J - \bar{J})^2} (G_0^{JJ} + G_0^{J\bar{J}}) \tag{99}$$

and thus

$$G_0^{JJ} + G_0^{J\bar{J}} = -\frac{6G_0^{pp} + 2c_1}{1 - 18p^4 V(\phi)^2/(J - \bar{J})^2}. \tag{100}$$

In these equations, also $G_0^{J\bar{J}} - G_0^{pp} = c_1$ has been used. Unlike in the Wheeler–DeWitt case, the remaining free function G_0^{pp} would not be fixed at the next order in the adiabatic expansion but through the second, quadratic constant C in (87).

We first verify that the fluctuations are at least positive as they should by definition. While this does not apply to G^{JJ} , \hat{J} not being self-adjoint, the quantity $G^{J+\bar{J}, J+\bar{J}} := \langle (\hat{J} + \hat{J}^\dagger)^2 \rangle - \langle \hat{J} + \hat{J}^\dagger \rangle^2$ must satisfy positivity conditions. Eq. (100) in fact shows that $G_0^{JJ} + G_0^{\bar{J}\bar{J}}$ is negative, and thus $G_0^{JJ} + G_0^{\bar{J}\bar{J}} + 6G_0^{pp} + 2c_1$ is positive from (99). This is relevant because the latter quantity can be written as $G^{JJ} + G^{\bar{J}\bar{J}} + 6G^{pp} + 2c_1 = G^{J+\bar{J}, J+\bar{J}} + 4G^{pp}$ in terms of the positive fluctuation $G^{J+\bar{J}, J+\bar{J}} := \langle (\hat{J} + \hat{J}^\dagger)^2 \rangle - \langle \hat{J} + \hat{J}^\dagger \rangle^2$ of the self-adjoint $\hat{J} + \hat{J}^\dagger$. The zeroth order adiabatic solutions are thus not in conflict with positivity of fluctuations.

Next, we check uncertainty relations. This time, there are several independent ones [15] because we are using partially complex basic variables. Independent uncertainty relations must then be fulfilled for each pair $(\hat{p}, \hat{J} + \hat{J}^\dagger)$, $(\hat{p}, i(\hat{J} - \hat{J}^\dagger))$ and $\hat{J} + \hat{J}^\dagger, i(\hat{J} - \hat{J}^\dagger)$ of self-adjoint operators. These relations, derived in [15], take the form

$$G^{pp}G^{J+\bar{J}, J+\bar{J}} - (G^{p, J+\bar{J}})^2 \geq -\frac{1}{4}\hbar^2(J - \bar{J})^2 \quad (101)$$

$$G^{pp}G^{i(J-\bar{J}), i(J-\bar{J})} - (G^{p, i(J-\bar{J})})^2 \geq \frac{1}{4}\hbar^2(J + \bar{J})^2 \quad (102)$$

$$G^{J+\bar{J}, J+\bar{J}}G^{i(J-\bar{J}), i(J-\bar{J})} - (G^{J+\bar{J}, i(J-\bar{J})})^2 \geq \hbar^2(2p + \hbar)^2. \quad (103)$$

The first one is easy to satisfy to this order since $G^{p, J+\bar{J}} = G^{pJ} + G^{p\bar{J}}$ vanishes. The left hand side of (101) is then positive as just shown, and one can find appropriate scalings (i.e. sufficiently large C) to ensure the uncertainty relation noting that $J - \bar{J}$ is nearly constant for perturbative solutions. The second relation is more difficult to verify since $G^{p, i(J-\bar{J})}$ is non-zero. For the zeroth order solutions, we have

$$G_0^{pp}G_0^{i(J-\bar{J}), i(J-\bar{J})} - (G_0^{p, i(J-\bar{J})})^2 = -G_0^{pp}(G_0^{JJ} + G_0^{\bar{J}\bar{J}} - 2G_0^{J\bar{J}}) + (G_0^{pJ} - G_0^{p\bar{J}})^2$$

which is at least positive since we saw that $G_0^{JJ} + G_0^{\bar{J}\bar{J}}$ is negative and $(G_0^{pJ} - G_0^{p\bar{J}})^2$, although negative, is of order $V(\phi)^2$ as a consequence of (98). Moreover, using the free solutions as a guide indicates that one might be able to satisfy the uncertainty relation: In the free case, we have

$$-(G_{V=0}^{JJ} + G_{V=0}^{\bar{J}\bar{J}} - 2G_{V=0}^{J\bar{J}}) = 2(c_1 - c_2) = 4(\Delta H)^2$$

which is positive and constant. With the factor of G^{pp} , which in the free case behaves as p^2 at least far away from the bounce one may have a chance to satisfy (102). Similarly, the third relation, which is simpler due to $G_0^{J+\bar{J}, i(J-\bar{J})} = i(G_0^{JJ} - G_0^{\bar{J}\bar{J}}) = 0$, has a left hand

side

$$\begin{aligned}
G_0^{J+\bar{J}, J+\bar{J}} G_0^{i(J-\bar{J}), i(J-\bar{J})} - (G_0^{J+\bar{J}, i(J-\bar{J})})^2 &= -(G_0^{JJ} + G_0^{\bar{J}\bar{J}})^2 + 4(G_0^{J\bar{J}})^2 \\
&= -\frac{(6G_0^{pp} + 2c_1)^2}{(1 - 18p^4 V(\phi)^2 / (J - \bar{J})^2)^2} + 4(G_0^{pp} + c_1)^2 \\
&= -32(G_0^{pp})^2 - 16c_1 G_0^{pp} - 144 \frac{p^4 V(\phi)^2}{(J - \bar{J})^2} (3G_0^{pp} + c_1)^2
\end{aligned}$$

for the first two leading orders in $p^2 V(\phi) / (J - \bar{J})$. It can be positive for states satisfying $c_1 < -2G_0^{pp}$, but also has to be larger than the ϕ -dependent $4\hbar^2 p^2$ as required by the uncertainty relation. A look at the free solutions also here indicates that this might be possible: both c_1 and $G_{V=0}^{pp}$ are of the order \hbar for saturation of the free uncertainty relations, and $G_{V=0}^{pp}$ behaves as p^2 far away from the bounce.

Using the candidate solutions for adiabatic quantum variables in the equation of motion for p then suggests an effective equation

$$\begin{aligned}
\dot{p} &= -\frac{J + \bar{J}}{2} + \frac{p^3(J + \bar{J})}{(J - \bar{J})^2} V(\phi) + 3 \frac{J + \bar{J}}{(J - \bar{J})^2} \left(1 - 8 \frac{p^3}{(J - \bar{J})^2}\right) G_0^{pp} V(\phi) \\
&\quad - 12 \frac{p^3(J + \bar{J})}{(J - \bar{J})^4} c_1 V(\phi) + 36 \frac{p^4(J + \bar{J})}{(J - \bar{J})^4} (3G_0^{pp} + c_1) V(\phi)^2
\end{aligned} \tag{104}$$

up to higher order terms in the potential. Here, c_1 is a constant parameterizing the state around which the effective equation is derived. Similarly, G_0^{pp} depends on c_1 and the second constant C in (87) which is preserved by the equations of motion we consider here. Thus, we would have an effective equation containing only two state dependent parameters but no free functions. However, in the final step of determining $G_0^{pp}(c_1, C)$ an inconsistency arises: using the candidate adiabatic solutions in (87) for a constant C , G_0^{pp} has to be constant up to perturbative terms of the order $p^4 V^2 / (J - \bar{J})^2$. However, we saw that the uncertainty relations require G_0^{pp} to behave as p^2 as it does in the free case. With a potential, there is no adiabatic regime in which this can be satisfied and the effective equation (104) is, after all, inconsistent.

3.3.3 Non-adiabaticity relative to free solutions

For the loop quantized model it is more complicated to introduce adiabaticity relative to free solutions because free quantum variables (27)–(32) are not simply proportional to powers of the expectation values as in the Wheeler–DeWitt case. The most direct possibility is to introduce the free solutions as explicitly time dependent functions $G_{V=0}^{a,n}(\phi)$. Resulting effective equations will then be strongly time dependent not just through the scalar potential. Then, for variables $g^{a,n} := G^{a,n} / G_{V=0}^{a,n}(\phi)$ and using (95)–(97) we have

equations of motion

$$\begin{aligned}
\dot{g}^{pp} &= - \left(1 - \frac{2p^3 V(\phi)}{(J - \bar{J})^2} \right) \left(\frac{G_{V=0}^{pJ}(\phi)}{G_{V=0}^{pp}(\phi)} g^{pJ} + \frac{G_{V=0}^{p\bar{J}}(\phi)}{G_{V=0}^{pp}(\phi)} g^{p\bar{J}} \right) + \frac{G_{V=0}^{pJ}(\phi) + G_{V=0}^{p\bar{J}}(\phi)}{G_{V=0}^{pp}(\phi)} g^{pp}, \\
\dot{g}^{pJ} &= - \frac{1}{2} \left(1 - \frac{2p^3 V(\phi)}{(J - \bar{J})^2} \right) \left(\frac{G_{V=0}^{JJ}(\phi)}{G_{V=0}^{pJ}(\phi)} g^{JJ} + \frac{G_{V=0}^{J\bar{J}}(\phi)}{G_{V=0}^{pJ}(\phi)} g^{J\bar{J}} + 2 \frac{G_{V=0}^{pp}(\phi)}{G_{V=0}^{pJ}(\phi)} g^{pp} \right) \\
&\quad + \frac{1}{2} \left(\frac{G_{V=0}^{JJ} + G_{V=0}^{J\bar{J}}(\phi) + 2G_{V=0}^{pp}(\phi)}{G_{V=0}^{pJ}(\phi)} + \frac{6p^2 V(\phi)}{J - \bar{J}} \right) g^{pJ} = \overline{\dot{g}^{p\bar{J}}}, \\
\dot{g}^{JJ} &= -2 \left(1 - \frac{2p^3 V(\phi)}{(J - \bar{J})^2} \right) \frac{G_{V=0}^{pJ}(\phi)}{G_{V=0}^{JJ}(\phi)} g^{pJ} + 2 \left(\frac{G_{V=0}^{pJ}(\phi)}{G_{V=0}^{JJ}(\phi)} + \frac{3p^2 V(\phi)}{J - \bar{J}} \right) g^{JJ} = \overline{\dot{g}^{J\bar{J}}}, \\
\dot{g}^{J\bar{J}} &= - \left(1 - \frac{2p^3 V(\phi)}{(J - \bar{J})^2} \right) \left(\frac{G_{V=0}^{pJ}(\phi)}{G_{V=0}^{J\bar{J}}(\phi)} g^{pJ} + \frac{G_{V=0}^{p\bar{J}}(\phi)}{G_{V=0}^{J\bar{J}}(\phi)} g^{p\bar{J}} \right) + \frac{G_{V=0}^{pJ}(\phi) + G_{V=0}^{p\bar{J}}(\phi)}{G_{V=0}^{J\bar{J}}(\phi)} g^{J\bar{J}}.
\end{aligned}$$

There is now a crucial difference to the situation in a Wheeler–DeWitt quantization as in Eqs. (65), (66) and (67): $V = 0$ is not a singular point for the adiabatic approximation. In the Wheeler–DeWitt equations, some terms completely vanish in the free case such that the solutions change dramatically. For instance, solving for g_0^{cp} requires one to divide by $V(\phi)$ which is not possible in the free case. Thus, the existence of consistent solutions satisfying uncertainty relations in the free case, and obviously being adiabatic for the variables $g^{a,n} = G^{a,n}/G_{V=0}^{a,n}(\phi) = 1$, does not guarantee the existence of consistent adiabatic solutions even under slight perturbations including a small potential. The equations obtained here for the loop quantization, on the other hand, are perfectly perturbative in $V(\phi)$ and the free solutions do not present a singular point for the adiabatic expansion.

Nevertheless, there are again no adiabatic solutions in the presence of a potential. While the linear system of six equations for six (real) variables at zeroth adiabatic order is degenerate when $V = 0$, allowing a non-trivial solution where all $g^{a,n} = 1$, the determinant of the coefficients can be seen to be non-vanishing for $V \neq 0$. Thus, the only solution in this case is $g^{a,n} = 0$ which again violates the uncertainty principles.

There might be adiabatic regimes for the equations (88)–(91) and (93)–(94) to this order, but this would be more involved and does not seem promising. We therefore turn to a new type of effective equations which does not require an adiabatic expansion.

4 Higher dimensional effective equations and perturbative solutions

Although our attempts to find adiabatic regimes and to solve for quantum variables in terms of expectation values were largely unsuccessful, prohibiting the derivation of effective equations solely in terms of expectation values, effective equations for an enlarged system do exist. Rather than solving for the fluctuations, we keep them as independent

variables in addition to the expectation values. This is still a system of classical type, given in terms of finitely many variables, since we already removed higher moments as part of the semiclassical expansion. But it is certainly different from the exact classical system not only in the form of its equations of motion but also by the number of independent variables. From a general viewpoint, this is in agreement with expectations from effective actions which generically give rise to higher derivative terms. Higher derivative actions imply higher derivative equations of motion which, when taken at face value, describe a larger set of independent degrees of freedom: additional parameters have to be specified for a complete initial value problem of higher derivative equations. However, when higher derivative terms arise from a perturbation expansion not all the solutions are consistent within this scheme. Only solutions analytic in the perturbation parameter are consistent, which can be shown to allow a number of independent solutions agreeing with the unperturbed case [27, 28]. Thus, higher derivative effective actions do not truly introduce new degrees of freedom. Keeping some of the quantum variables, on the other hand, requires additional initial conditions even for perturbative solutions; in this case new quantum degrees of freedom truly arise.

4.1 Wheeler–DeWitt model

In variables c and p , we thus have a set of five coupled effective equations

$$\begin{aligned}
\dot{c} &= c + \left(-\frac{p}{c} - \frac{p}{c^3} G^{cc} + \frac{1}{c^2} G^{cp} \right) V(\phi) \\
\dot{p} &= -p + \left(-\frac{p^2}{2c^2} - \frac{3p^2}{2c^4} G^{cc} + \frac{2p}{c^3} G^{cp} - \frac{1}{2c^2} G^{pp} \right) V(\phi) \\
\dot{G}^{cc} &= 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G^{cc} - \frac{2}{c} G^{cp} V(\phi) \\
\dot{G}^{cp} &= \left(\frac{p^2}{c^3} G^{cc} - \frac{1}{c} G^{pp} \right) V(\phi) \\
\dot{G}^{pp} &= \frac{2p^2}{c^3} G^{cp} V(\phi) - 2 \left(1 + \frac{p}{c^2} V(\phi) \right) G^{pp}.
\end{aligned} \tag{105}$$

Back-reaction terms of fluctuations are included in the equations of motion for expectation values, although the role of an effective potential is illustrated more indirectly than it would be for adiabatic effective equations.

For perturbations around free solutions, assuming small values of the potential $V(\phi) = \epsilon \mathcal{V}(\phi)$ with a small parameter ϵ , we define

$$p(\phi) = p_0(\phi) + \epsilon p_1(\phi) + \dots \tag{106}$$

and similarly for the other variables, where p_0 is the zeroth order solution (13) corresponding to $V(\phi) = 0$. (For simplicity we now use a simple zero as subscript for the free solutions rather than “ $V = 0$ ”. Confusion will not arise because the adiabatic approximation will no

longer be used.) All free solutions are explicitly given by (12)–(16). To first perturbative order in ϵ , the equations of motion (105) become

$$\begin{aligned}
\dot{c}_1 &= c_1 + \left(-\frac{p_0}{c_0} - \frac{p_0}{c_0^3} G_0^{cc} + \frac{1}{c_0^2} G_0^{cp} \right) \mathcal{V}(\phi) \\
\dot{p}_1 &= -p_1 + \left(-\frac{1}{2} \frac{p_0^2}{c_0^2} - \frac{3p_0^2}{2c_0^4} G_0^{cc} + 2\frac{p_0}{c_0^3} G_0^{cp} - \frac{1}{2c_0^2} G_0^{pp} \right) \mathcal{V}(\phi) \\
\dot{G}_1^{cc} &= 2G_1^{cc} + 2 \left(\frac{p_0}{c_0^2} G_0^{cc} - \frac{1}{c_0} G_0^{cp} \right) \mathcal{V}(\phi) \\
\dot{G}_1^{cp} &= \left(\frac{p_0^2}{c_0^3} G_0^{cc} - \frac{1}{c_0} G_0^{pp} \right) \mathcal{V}(\phi) \\
\dot{G}_1^{pp} &= -2G_1^{pp} + 2 \left(\frac{p_0^2}{c_0^3} G_0^{cp} - \frac{p_0}{c_0^2} G_0^{pp} \right) \mathcal{V}(\phi)
\end{aligned} \tag{107}$$

which are inhomogeneous differential equations whose homogeneous terms are linear. Proceeding in the same way to higher orders, this provides a well-defined and self-consistent solution scheme for the interacting dynamics of the quantum system. There are two expansions of the full quantum equations: a semiclassical one (truncating higher moments) and the perturbative one in ϵ (removing higher powers of the potential). When extending to higher orders, one would thus have to find out what the relative magnitudes of correction terms in the different expansions are.

Using the free solutions (12)–(16) for the different variables we obtain the perturbative solutions up to first order in ϵ :

$$\begin{aligned}
c_1(\phi) &= B_1 e^\phi + (C_2/C_1 + C_2 C_3/C_1^3 - C_4/C_1^2) e^\phi \int^\phi \mathcal{V}(\tau) e^{-3\tau} d\tau \\
p_1(\phi) &= B_2 e^{-\phi} - (-C_2^2/2C_1^2 - 3C_2^2 C_3/2C_1^4 + 2C_2 C_4/C_1^3 - C_5/2C_1^2) e^{-\phi} \int^\phi \mathcal{V}(\tau) e^{-3\tau} d\tau \\
G_1^{cc}(\phi) &= B_3 e^{2\phi} - 2(C_2 C_3/C_1^2 - C_4/C_1) e^{2\phi} \int^\phi \mathcal{V}(\tau) e^{-3\tau} d\tau \\
G_1^{cp}(\phi) &= B_4 - (C_2^2 C_3/C_1^3 - C_5/C_1) \int^\phi \mathcal{V}(\tau) e^{-3\tau} d\tau \\
G_1^{pp}(\phi) &= B_5 e^{-2\phi} - 2(C_2^2 C_4/C_1^3 - C_2 C_5/C_1^2) e^{-2\phi} \int^\phi \mathcal{V}(\tau) e^{-3\tau} d\tau
\end{aligned}$$

where (B_1, \dots, B_5) are further constants of integration simply adding up to the zeroth order constants in (12)–(16). Specifically, for a mass term potential $V(\phi) = \frac{1}{2} m^2 \phi^2 = \epsilon \phi^2$

we have

$$\begin{aligned}
c_1(\phi) &= B_1 e^\phi + \frac{1}{27}(C_2/C_1 + C_2 C_3/C_1^3 - C_4/C_1^2)(2 + 6\phi + 9\phi^2)e^{-2\phi} \\
p_1(\phi) &= B_2 e^{-\phi} - \frac{1}{27}(-C_2^2/2C_1^2 - 3C_2^2 C_3/2C_1^4 + 2C_2 C_4/C_1^3 - C_5/2C_1^2)(2 + 6\phi + 9\phi^2)e^{-4\phi} \\
G_1^{cc}(\phi) &= B_3 e^{2\phi} - \frac{2}{27}(C_2 C_3/C_1^2 - C_4/C_1)(2 + 6\phi + 9\phi^2)e^{-\phi} \\
G_1^{cp}(\phi) &= B_4 - \frac{1}{27}(C_2^2 C_3/C_1^3 - C_5/C_1)(2 + 6\phi + 9\phi^2)e^{-3\phi} \\
G_1^{pp}(\phi) &= B_5 e^{-2\phi} - \frac{2}{27}(C_2^2 C_4/C_1^3 - C_2 C_5/C_1^2)(2 + 6\phi + 9\phi^2)e^{-5\phi}.
\end{aligned}$$

These solutions already display interesting properties of the system. Compared to the free solutions which are pure exponentials in ϕ , there are different types of corrections. Since we are perturbatively adding a potential one certainly expects corrections to the solutions which correspond to some of the polynomial terms. For the classical variables c and p , these agree with corrections to the classical solutions resulting from the potential. But there are additional corrections displaying genuine quantum behavior since fluctuations $G^{a,2}$ evolve, too, and couple to the expectation values. Although they are structurally similar, one can easily disentangle both types of corrections by setting the zeroth order fluctuations to zero. (This is not possible for the quantum system since it would violate uncertainty relations. But we are free to do so formally to discuss different correction terms.) Zeroth order fluctuations are zero if we set $C_3 = C_4 = C_5 = 0$. This removes some corrections from c_1 and p_1 which can therefore be attributed unambiguously to quantum back-reaction. They differ from classical corrections only in their coefficients, related to the integration constants. The time dependence of the correction, in this model, is thus the same as the classical one and quantum back-reaction does not change the expectation values significantly. Moreover, their coefficients are small if a state is semiclassical at large volume, which requires that the fluctuation parameters C_3 , C_4 and C_5 are small compared to C_1 and C_2 .

4.2 Loop quantization

The loop quantization, being formulated in non-canonical variables (p, J) , leads to a different algebra of expectation values and quantum variables. Moreover, due to the use of the complex variable J , which is typical for loop quantization based on holonomies, there are more independent variables and equations of motion. This is supplemented by a reality condition (26) which leaves the correct number of degrees of freedom when implemented. The Poisson brackets (70)–(77) together with the quantum Hamiltonian (68) result in equations of motion (88) and (89). With equations of motion (90), (91), (93) and (94) for $\dot{G}^{a,2}$, this provides our higher dimensional effective system of the loop quantization.

For perturbative solutions of the expectation values we expand as in (106), use free solutions $p_0(\phi)$, $J_0(\phi)$ and $G_0^{a,2}(\phi)$ from (12)–(16) on the right hand side and integrate. We

do not require solutions or even equations of motion for $G_1^{a,2}$ to this order in a perturbative solution scheme if we are only interested in $p_1(\phi)$ to analyze the bounce. Strictly speaking, G_1^{pp} and $G_1^{J\bar{J}}$ are also necessary to implement the reality condition, but we can avoid explicit solutions since we already verified that the reality condition is preserved under evolution generated by our truncated quantum Hamiltonian. The evolution of $G_1^{J\bar{J}} - G_1^{pp}$, however, will be considered below to analyze effects of the reality condition on the bounce.

For the real part of J which couples to p , the equations give

$$\begin{aligned}
\frac{1}{2}(J + \bar{J})\dot{} &= -(p + \hbar/2) + \frac{3}{2}p^2V(\phi) + 2\frac{p^3(p + \hbar/2)}{(J - \bar{J})^2}V(\phi) \\
&+ \left(\frac{3p^2}{2(J - \bar{J})^2} + \frac{6p^3(p + \hbar/2)}{(J - \bar{J})^4} \right) (G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}})V(\phi) \\
&- 3 \left(\frac{p}{J - \bar{J}} + \frac{4p^2(p + \hbar/2)}{(J - \bar{J})^3} \right) (G^{pJ} - G^{p\bar{J}})V(\phi) \\
&+ \frac{3}{2} \left(1 + \frac{4p(p + \hbar/2)}{(J - \bar{J})^2} \right) G^{pp}V(\phi) \\
&+ \frac{p}{(J - \bar{J})^3} (3(J - \bar{J})^2 - 4p^2) (G^{pJ} - G^{p\bar{J}})V(\phi) \\
&- \frac{3}{2} \frac{p^2}{(J - \bar{J})^2} (G^{JJ} + G^{\bar{J}\bar{J}} - 2G^{J\bar{J}} - 4G^{pp})V(\phi).
\end{aligned} \tag{108}$$

Zeroth order solutions (27)–(32) for this system now describe bouncing cosmologies. They satisfy $J_0 - \bar{J}_0 = 2iH_0$ which is the constant free Hamiltonian, and $G_0^{JJ} + G_0^{\bar{J}\bar{J}} - 2G_0^{J\bar{J}} = 2(c_2 - c_1)$ (with $c_1 - c_2 = 2(\Delta H_0)^2 > 0$) which can be used to simplify some calculations. Perturbed equations of motion are more complicated than for the Wheeler–DeWitt model, but we can focus on a few dominant terms. Moreover, we can assume $A = B$ in (27), (28) since we would just need to shift our internal time otherwise. We keep the classical perturbation, given by $p^3(J - \bar{J})^{-2}V(\phi)$ for \dot{p} and $\frac{3}{2}p^2V(\phi) + 2p^3(p + \hbar/2)(J - \bar{J})^{-2}V(\phi)$ for $\frac{1}{2}(J + \bar{J})\dot{}$, which contributes (considering only the highest positive and negative exponents)

$$-\frac{J_0 + \bar{J}_0}{4H_0^2}p_0^3 \sim -A^4 \frac{e^{-4\phi} - e^{4\phi}}{32H_0^2}$$

to \dot{p}_1 and

$$-\frac{p_0^2}{8H_0^2}(4p_0^2 - 3H_0^2) \sim -A^4 \frac{e^{-4\phi} + e^{4\phi}}{32H_0^2}$$

to $\frac{1}{2}(J_1 + \bar{J}_1)\dot{}$. This is to be compared with the quantum correction term having the strongest time dependence, which turns out to be

$$\frac{1}{16} \frac{A^2}{H_0^2} \left(\left(\frac{3}{4} \frac{A^2}{H_0^2} (c_2 - c_1) - 6c_3 + 4 \frac{A}{H_0} c_6 \right) e^{-4\phi} - \left(\frac{3}{4} \frac{A^2}{H_0^2} (c_2 - c_1) - 6c_4 + 4 \frac{A}{H_0} c_5 \right) e^{4\phi} \right)$$

for \dot{p} and

$$\frac{1}{16} \frac{A^2}{H_0^2} \left(\left(\frac{3}{4} \frac{A^2}{H_0^2} (c_2 - c_1) - 6c_3 + 4 \frac{A}{H_0} c_6 \right) e^{-4\phi} + \left(\frac{3}{4} \frac{A^2}{H_0^2} (c_2 - c_1) - 6c_4 + 4 \frac{A}{H_0} c_5 \right) e^{4\phi} \right)$$

for $\frac{1}{2}(J + \bar{J})$. The inhomogeneous linear differential equations for the first order perturbations are solved by

$$\begin{aligned} p_1(\phi) &= \frac{1}{2}(A_1(\phi)e^{-\phi} + B_1(\phi)e^{\phi}) \\ \frac{1}{2}(J_1(\phi) + \bar{J}_1(\phi)) &= \frac{1}{2}(A_1(\phi)e^{-\phi} - B_1(\phi)e^{\phi}) \end{aligned}$$

with

$$\begin{aligned} \dot{A}_1(\phi) &= -\frac{A^2}{16H_0^2}\mathcal{V}(\phi) \left(A^2 - \frac{3}{2}\frac{A^2}{H_0^2}(c_2 - c_1) + 12c_3 - 8\frac{A}{H_0}c_6 \right) e^{-3\phi} \\ \dot{B}_1(\phi) &= -\frac{A^2}{16H_0^2}\mathcal{V}(\phi) \left(A^2 - \frac{3}{2}\frac{A^2}{H_0^2}(c_2 - c_1) + 12c_4 - 8\frac{A}{H_0}c_5 \right) e^{3\phi} \end{aligned}$$

for the perturbative potential again defined as $V(\phi) = \epsilon\mathcal{V}(\phi)$. Thus,

$$\begin{aligned} p_1(\phi) &= \frac{A^4}{32H_0^2} \left(1 - \frac{3}{2}\frac{c_2 - c_1}{H_0^2} \right) \left(e^{\phi} \int^{\phi} \mathcal{V}(y)e^{3y}dy - e^{-\phi} \int^{\phi} \mathcal{V}(y)e^{-3y}dy \right) \\ &\quad + \frac{3}{8}\frac{A^2}{H_0^2}\alpha_1 \left(e^{\phi-\delta_1} \int^{\phi} \mathcal{V}(y)e^{3y}dy - e^{-\phi+\delta_1} \int^{\phi} \mathcal{V}(y)e^{-3y}dy \right) \\ &\quad - \frac{1}{4}\frac{A^2}{H_0^2}\alpha_2 \left(e^{\phi-\delta_2} \int^{\phi} \mathcal{V}(y)e^{3y}dy - e^{-\phi+\delta_2} \int^{\phi} \mathcal{V}(y)e^{-3y}dy \right) \end{aligned} \quad (109)$$

with

$$\alpha_1 = \sqrt{c_3c_4} \quad , \quad \alpha_2 = \sqrt{c_5c_6} \quad , \quad e^{2\delta_1} = \frac{c_3}{c_4} \quad , \quad e^{2\delta_2} = \frac{c_6}{c_5}. \quad (110)$$

(Integration constants from integrating $A_1(\phi)$ and $B_1(\phi)$ can be absorbed in the zeroth order ones.) The parameters δ_I are related to the squeezing of the unperturbed state, with $\delta_I = 0$ for an unsqueezed state [15].

To this perturbative order, the bounce persists even under inclusion of a matter potential. As in the free model, the key to deciding whether or not there is a bounce, i.e. whether or not p is bounded away from zero, is the reality condition (26). In the free case, its implementation resulted in selecting the cosh-solution for p and ruling out the sinh solution, proving the bounce under the assumption of a semiclassical state at large volume. (The integration constants A and B must have equal sign in (27) if c_1 is not too large and negative.) Perturbatively, the reality condition becomes

$$\begin{aligned} \frac{1}{4}\hbar^2 &= |J|^2 - (p + \hbar/2)^2 - G^{pp} + G^{J\bar{J}} = |J_0|^2 - (p_0 + \hbar/2)^2 + c_1 \\ &\quad + 2\epsilon \left(\text{Re}J_0\text{Re}J_1 + \text{Im}J_0\text{Im}J_1 - (p_0 + \hbar/2)p_1 - \frac{1}{2}G_1^{pp} + \frac{1}{2}G_1^{J\bar{J}} \right) + O(\epsilon^2). \end{aligned} \quad (111)$$

The zeroth order is already implemented by starting with the correct zeroth order solutions. The linear order can then be seen to be automatically satisfied as well, such that the bouncing behavior at zeroth order is not affected by the perturbation.

It is, however, also clear that the bounce, with its mixture of collapsing and expanding functions, leads to stronger quantum back-reaction than classically. Although α_1 and α_2 are small compared to H_0^2 for a state which starts out semiclassically, depending on the values of δ_1 and δ_2 there can be exponential magnifications. For $c_3 \approx c_4$ and $c_5 \approx c_6$, which corresponds to nearly unsqueezed states and implies fluctuations nearly symmetric around the bounce point [15] quantum corrections are still small at the bounce if they were small for an initial solution. But for squeezed states with c_3 differing from c_4 corrections can be noticeable even earlier, before the bounce. This is illustrated by the solution

$$\begin{aligned}
G_1^{J\bar{J}} - G_1^{pp} = & \frac{1}{36} \frac{A^3}{H_0^2} (c_1 - c_2) ((2 + 9\phi^2) \cosh(3\phi) - 6\phi \sinh(3\phi)) \\
& - \frac{1}{108} \frac{A^4}{H_0^3} (c_5 - c_6) ((2 + 9\phi^2) \sinh(3\phi) - 6\phi \cosh(3\phi)) \\
& - \frac{1}{36} \frac{A^3}{H_0^2} \left(4 \frac{H_0^2}{A^2} - 1 \right) \alpha_1 ((2 + 9\phi^2) \cosh(3\phi - \delta_1) - 6\phi \sinh(3\phi - \delta_1)) \\
& + \frac{1}{12} \frac{A^2}{H_0} \alpha_2 ((2 + 9\phi^2) \cosh(3\phi - \delta_2) - 6\phi \sinh(3\phi - \delta_2))
\end{aligned} \tag{112}$$

for the combination of fluctuations featuring in the reality condition (specializing to a quadratic potential $\mathcal{V}(\phi) = \phi^2$). Especially the sign of this combination is important since a large negative value can push the bounce in the deep quantum regime even for large H . We have $c_1 - c_2 = 2(\Delta H_0)^2 > 0$ for the energy fluctuation of free solutions. If we use $A \approx H_0$ which, as a consequence of the reality condition, is satisfied for free solutions with large H_0 and assume unsqueezed states $c_3 \approx c_4$, $c_5 \approx c_6$ and put the extra condition $c_3 \approx c_5$, the remaining terms cancel and $G_1^{J\bar{J}} - G_1^{pp}$ is positive. But for squeezed states there can be significant contributions from fluctuations at the bounce, which can even make $G_1^{J\bar{J}} - G_1^{pp}$ negative there. In such a situation, it is important to know the precise state, i.e. all parameters c_1 , c_2 , α_1 , α_2 , δ_1 and δ_2 , in order to determine the quantum nature of the bounce. However, the relevant squeezing parameters cannot be fully determined from using the state at only one side of the bounce [29] due to exponential suppression factors of some of the integration constants in (29)–(32) if one restricts ϕ to a fixed sign. Thus, the precise quantum nature of the bounce may always depend on what assumptions one makes for a state.

5 Conclusions

Loop quantum cosmology implements the discrete nature of quantum gravity, in contrast to Wheeler–DeWitt quantum cosmology. Its dynamics is determined by a difference, rather than differential equation, resulting in singularity-free solutions by general arguments in symmetric models [7, 8]. But in general no intuitive geometrical picture for the avoidance of the classical big bang singularity is provided; typically the regime around a classical singularity is of a highly quantum nature. Nevertheless, such regimes may be probed by

effective equations, a first example being presented in [10]. Surprisingly, a very smooth bounce picture resulted in the model studied there (an isotropic cosmology sourced by a free, massless scalar), with the whole history described well by simply replacing a connection component c in the Hamiltonian constraint by $\sin c$. This replacement is motivated by the use of holonomies, rather than connection components themselves, in loop quantum gravity. But there are undoubtedly other corrections in a general quantum system as well as other types of corrections expected from a loop quantization, and it was unexpected that only the holonomy replacement provides effective equations in a precise manner. These equations were indeed shown to be effective equations in a strict sense [14] since other quantum corrections in this specific model are simply absent. But this analysis also showed that the validity of effective equations obtained by the holonomy replacement is very special and tied to the free scalar model.

In this paper, we have provided a detailed systematic analysis for massive or self-interacting scalars. The situation turns out to be remarkably different from the free scalar models: back-reaction of fluctuations on expectation values cannot be ignored, giving rise to extra quantum corrections to the classical equations. Moreover, standard as well as more involved choices of setting up an adiabatic approximation of fluctuations were unsuccessful in that the adiabaticity assumption was in conflict either with uncertainty relations or did not lead to any complete solution to all equations of motion. Thus, for the cases analyzed here there is no analog of a low-energy effective action. There may be regimes where an adiabaticity assumption is consistent, but this had to be rather contrived. Our conclusion is that in general only higher dimensional effective systems exist for quantum cosmology, which crucially contain independent quantum degrees of freedom. In particular, the holonomy replacement of c by $\sin c$ in loop quantum cosmology is not sufficient, although it still occurs due to the use of $J = pe^{ic}$ as basic variable in the setup of effective equations.

In general, the holonomy replacement by itself overlooks crucial quantum effects caused by back-reactions of a spreading and deforming state on its expectation values. (This can be seen as a crude way of writing effective equations by setting $G^{a,n} = 0$, which obviously violates uncertainty relations.) This is important to realize since the replacement has often occurred in the recent literature, see e.g. [30, 6, 31, 32, 33]. It is used either in the form of $\sin c$ in the Friedmann equation, or by using equations of motion to solve $\sin c$ in terms of \dot{a} , which gives rise to a correction term of energy density squared to the classical Friedmann equation [30]: starting from a Hamiltonian constraint of the form $C = -\mu^{-2} \sin^2(\mu c) \sqrt{|p|} + |p|^{3/2} \rho_{\text{matter}}$ (where μ may be a p -dependent function) one derives the Hamiltonian equation of motion $\dot{p} = 2\mu^{-1} \sin(\mu c) \cos(\mu c) \sqrt{|p|}$. From $|p| = a^2$, on the other hand, we have $\dot{p} = 2a\dot{a}$ such that the constraint $C = 0$ can be expressed as the corrected Friedmann equation

$$\dot{a}^2 = \mu^{-2} \sin^2(\mu c) (1 - \sin^2(\mu c)) = a^2 \rho_{\text{matter}} (1 - (\mu a)^2 \rho_{\text{matter}}) \quad (113)$$

using $C = 0$. This equation looks very suggestive and easily generalizable to arbitrary matter densities, which in fact has often been done in the recent past. However, this equation is applicable only to an exactly isotropic model sourced by a *free, massless scalar*. Even

before embarking on a systematic analysis of effective equations as in this paper, the holonomy replacement $\sin c$ could not be expressed simply as a ρ^2 -correction (or possibly higher power) if anisotropies or inhomogeneities are included. Then, several independent gravitational variables exist and one cannot simply solve for a single \dot{a} to bring the gravitational part of the Friedmann equation in classical form and have only the matter contribution corrected.

Moreover, our analysis has shown that the holonomy replacement is not the only quantum correction when matter interactions are allowed for. (Similar effects happen when anisotropies or inhomogeneities are included in addition to the complications for solving for \dot{a} mentioned above.) Quantum fluctuation terms are not only to be included in the effective equations but even to be kept as independent variables.³ The replacement of c by $\sin c$ by itself does not result in proper effective equations at all; such equations are rather to be considered *phenomenological* by isolating one quantum effect but ignoring others. (A similar type of phenomenological equations without proper effective analysis occurred in [34] as the first such example in loop quantum cosmology.) Studies of such phenomenological equations are valuable, but to avoid misunderstanding they should be clearly designated as “phenomenological” rather than “effective” unless an analysis of proper quantum aspects has been performed.

Compared to corrections from inverse powers of metric components, which were utilized in [34] and elsewhere, for higher order corrections in c as they result from the holonomy replacement it is more important to keep fluctuation terms. Both are related to higher curvature corrections (higher powers of a time derivatives of metric components on the one hand and higher order time derivatives on the other) as they are usually expected from effective actions. These corrections are better not to be separated, or else violations of covariance may easily occur.

Proper effective equations for flat isotropic models sourced by *massive or self-interacting scalars* have been provided here to first order in \hbar , provided by moments of second order. We have seen higher powers of c playing a role in the variable J , which also enters equations of motion. In addition, there are clearly quantum degrees of freedom corresponding to independent fluctuations in the effective equations. This is in agreement with expectations from higher curvature terms, although not in obvious correspondence. In our case, we have true independent quantum degrees of freedom even at the perturbative level, while higher derivatives in effective actions do not provide new degrees of freedom as independent solutions in a consistent perturbation scheme.

We have analyzed the effective equations perturbatively, making sure that reality conditions are respected. The solutions correspond to moments computed from a physically normalized state. At first perturbative order, there is no strong back-reaction for a Wheeler–DeWitt quantization, or for most of a single collapsing or expanding branch in a loop quantization. But quantum back-reaction effects are noticeable for squeezed states around

³Even if they were included in the effective potential, matter terms themselves would be c -dependent, and (113) would only be an implicit equation for \dot{a} whose properties would differ from an explicit one with a \dot{a} -independent right hand side in (113).

the bounce of loop quantum cosmology due to the influence of the growing branch on the collapsing one. Since squeezing parameters of a bouncing state are not determined by properties in one of the two large volume regime only [29], no general statement about the presence of a semiclassical bounce is available. There are quantum parameters whose influence is negligible at large volume but which will become important near a bounce and determine its fate. This shows the caution required for statements about the behavior of a bounce even in a perturbative regime around the exact bounce model. While a full analysis is beyond the scope of this paper, we have provided the setting based on a proper derivation and analysis of effective equations.

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A Poisson brackets between fluctuations in loop quantum cosmology

Here we provide more information on the derivation of Poisson brackets (78) – (86). All derivations follow the same scheme, except for (78) which does not give rise to third order moments because $[\hat{J}\hat{J}^\dagger, \hat{p}^2] = 0 = [\hat{J}^\dagger\hat{J}, \hat{p}^2]$. In this case, we have

$$\begin{aligned} \{G^{pp}, G^{J\bar{J}}\} &= \frac{1}{2}\{\langle\hat{p}^2 - p^2\rangle, \langle\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J} - 2J\bar{J}\rangle\} \\ &= \frac{1}{2i\hbar}\langle[\hat{p}^2, \hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}]\rangle - \frac{1}{i\hbar}J\langle[\hat{p}^2, \hat{J}^\dagger]\rangle - \frac{1}{i\hbar}\bar{J}\langle[\hat{p}^2, \hat{J}]\rangle - \frac{1}{i\hbar}p\langle[\hat{p}, \hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}]\rangle \\ &\quad + \{p^2, J\bar{J}\} \\ &= -iJ\langle\hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}\rangle + i\bar{J}\langle\hat{p}\hat{J} + \hat{J}\hat{p}\rangle = -2i(JG^{p\bar{J}} - \bar{J}G^{pJ}). \end{aligned}$$

For the remaining brackets there are contributions by moments of third order such as

$$\begin{aligned} G^{pJJ} &:= \frac{1}{3}\langle(\hat{p} - p)(\hat{J} - J)^2 + (\hat{J} - J)(\hat{p} - p)(\hat{J} - J) + (\hat{J} - J)^2(\hat{p} - p)\rangle \\ &= \frac{1}{3}\langle\hat{p}\hat{J}^2 + \hat{J}\hat{p}\hat{J} + \hat{J}^2\hat{p} - 3p\hat{J}^2 - 3J(\hat{p}\hat{J} + \hat{J}\hat{p}) + 6pJ\hat{J} + 3J^2\hat{p} - 3pJ^2\rangle \\ &= \frac{1}{3}\langle\hat{p}\hat{J}^2 + \hat{J}\hat{p}\hat{J} + \hat{J}^2\hat{p}\rangle - 2J(G^{pJ} + pJ) - p(G^{JJ} + J^2) + 2pJ^2 \\ &= \frac{1}{2}\langle\hat{p}\hat{J}^2 + \hat{J}^2\hat{p}\rangle - 2JG^{pJ} - pG^{JJ} - pJ^2 \end{aligned} \tag{114}$$

where we used $\hat{J}\hat{p}\hat{J} = \frac{1}{2}(\hat{p}\hat{J}^2 + \hat{J}^2\hat{p})$. We will also use the third moment

$$G^{ppJ} = \frac{1}{3}\langle\hat{p}^2\hat{J} + \hat{p}\hat{J}\hat{p} + \hat{J}\hat{p}^2\rangle - 2p(G^{pJ} + pJ) - J(G^{pp} + p^2) + 2p^2J \tag{115}$$

obtained by a similar calculation, or just by exchanging p and J in G^{pJJ} . (But note that the final step in (114) does differ since we now have

$$\hat{p}\hat{J}\hat{p} = \frac{1}{2}(\hat{p}(\hat{p}\hat{J} - \hbar\hat{J}) + (\hat{J}\hat{p} + \hbar\hat{J})\hat{p}) = \frac{1}{2}(\hat{p}^2\hat{J} + \hat{J}\hat{p}^2 - \hbar[\hat{p}, \hat{J}]) = \frac{1}{2}(\hat{p}^2\hat{J} + \hat{J}\hat{p}^2 - \hbar^2\hat{J}). \quad (116)$$

This allows us to express the Poisson brackets between fluctuations in terms of moments and expectation values:

$$\begin{aligned} \{G^{pp}, G^{JJ}\} &= \frac{1}{i\hbar}\langle[\hat{p}^2, \hat{J}^2]\rangle - \frac{2}{i\hbar}J\langle[\hat{p}^2, \hat{J}]\rangle - \frac{2}{i\hbar}p\langle[\hat{p}, \hat{J}^2]\rangle + \{p^2, J^2\} \\ &= -2i\langle\hat{p}\hat{J}^2 + \hat{J}^2\hat{p}\rangle + 2iJ\langle\hat{p}\hat{J} + \hat{J}\hat{p}\rangle + 4ip\langle\hat{J}^2\rangle - 4ipJ^2 \\ &= -4iG^{pJJ} - 4iJG^{pJ} \end{aligned}$$

using (114) in the last step. Furthermore, we obtain

$$\begin{aligned} \{G^{pp}, G^{pJ}\} &= \frac{1}{2i\hbar}\langle[\hat{p}^2, \hat{p}\hat{J} + \hat{J}\hat{p}]\rangle - \frac{1}{i\hbar}p\langle[\hat{p}^2, \hat{J}]\rangle - \frac{1}{i\hbar}p\langle[\hat{p}, \hat{p}\hat{J} + \hat{J}\hat{p}]\rangle + \{p^2, pJ\} \\ &= -\frac{1}{2}i\langle\hat{p}^2\hat{J} + 2\hat{p}\hat{J}\hat{p} + \hat{J}\hat{p}^2\rangle + 2ip\langle\hat{p}\hat{J} + \hat{J}\hat{p}\rangle - 2ip^2J \\ &= -\frac{2}{3}i\langle\hat{p}^2\hat{J} + \hat{p}\hat{J}\hat{p} + \hat{J}\hat{p}^2\rangle + \frac{1}{6}i\hbar^2J + 4ip(G^{pJ} + pJ) - 2ip^2J \\ &= -2iG^{ppJ} - 2iJG^{pp} + \frac{1}{6}i\hbar^2J \end{aligned}$$

where we used (116) to bring the third moment in the form as it appears in (115). The remaining brackets follow from similar calculations, although they can become more lengthy if all three basic operators \hat{p} , \hat{J} and \hat{J}^\dagger are involved. Skipping some of the details of calculational steps already encountered, and occasionally using the commutation relations as well as $\hat{J}\hat{J}^\dagger = \hat{p}^2$ and the associated reality condition (26), we further have

$$\begin{aligned} \{G^{JJ}, G^{JJ}\} &= \frac{1}{2i\hbar}\langle[\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}, \hat{J}^2]\rangle - \frac{1}{i\hbar}J\langle[\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}, \hat{J}]\rangle - \frac{1}{i\hbar}J\langle[\hat{J}^\dagger, \hat{J}^2]\rangle + \{JJ, J^2\} \\ &= -i\langle\hat{J}^2\hat{p} + 2\hat{J}\hat{p}\hat{J} + \hat{p}\hat{J}^2 + 2\hbar\hat{J}^2\rangle + 4iJ\langle\hat{p}\hat{J} + \hat{J}\hat{p}\rangle - 4ipJ^2 + 2i\hbar J^2 \\ &= -4iG^{pJJ} - 8iJ(G^{pJ} + pJ) - 4ip(G^{JJ} + JJ) + 8ipJ^2 - 2i\hbar(G^{JJ} + J^2) \\ &\quad + 8iJ(G^{pJ} + pJ) - 4ipJ^2 + 2i\hbar J^2 = -4iG^{pJJ} - 4i(p + \hbar/2)G^{JJ}, \end{aligned}$$

$$\begin{aligned} \{G^{JJ}, G^{pJ}\} &= \frac{1}{4i\hbar}\langle[\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}, \hat{p}\hat{J} + \hat{J}\hat{p}]\rangle - \frac{1}{2i\hbar}p\langle[\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}, \hat{J}]\rangle - \frac{1}{2i\hbar}J\langle[\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}, \hat{p}]\rangle \\ &\quad - \frac{1}{2i\hbar}J\langle[\hat{J}^\dagger, \hat{p}\hat{J} + \hat{J}\hat{p}]\rangle - \frac{1}{2i\hbar}\bar{J}\langle[\hat{J}, \hat{p}\hat{J} + \hat{J}\hat{p}]\rangle + \{JJ, pJ\} \\ &= -\frac{1}{2}i\langle\hat{p}^2\hat{J} + 2\hat{p}\hat{J}\hat{p} + \hat{J}\hat{p}^2\rangle + i(p + \hbar)\langle\hat{p}\hat{J} + \hat{J}\hat{p}\rangle + 2i\hbar pJ + 2iJ\langle\hat{p}^2\rangle \\ &\quad + \frac{1}{2}iJ\langle\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}\rangle - i\bar{J}\langle\hat{J}^2\rangle - 2ip(p + \hbar/2)J \\ &= -2iG^{ppJ} - 2i(p + \hbar/2)G^{pJ} + iJG^{JJ} - i\bar{J}G^{JJ} + \frac{1}{6}i\hbar^2J, \end{aligned}$$

$$\begin{aligned}
\{G^{JJ}, G^{pJ}\} &= \frac{1}{2i\hbar} \langle [\hat{J}^2, \hat{p}\hat{J} + \hat{J}\hat{p}] \rangle - \frac{1}{i\hbar} J \langle [\hat{J}^2, \hat{p}] \rangle - \frac{1}{i\hbar} J \langle [\hat{J}, \hat{p}\hat{J} + \hat{J}\hat{p}] \rangle + \{J^2, pJ\} \\
&= 2i\langle \hat{J}^3 \rangle - 4iJ\langle \hat{J}^2 \rangle + 2iJ^3 = 2iG^{JJJ} + 2iJG^{JJ},
\end{aligned}$$

$$\begin{aligned}
\{G^{JJ}, G^{p\bar{J}}\} &= \frac{1}{2i\hbar} \langle [\hat{J}^2, \hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}] \rangle - \frac{1}{i\hbar} \bar{J} \langle [\hat{J}^2, \hat{p}] \rangle - \frac{1}{i\hbar} J \langle [\hat{J}, \hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}] \rangle + \{J^2, p\bar{J}\} \\
&= 2i\langle \hat{p}^2\hat{J} + \hat{p}\hat{J}\hat{p} + \hat{J}\hat{p}^2 + 2\hbar(\hat{p}\hat{J} + \hat{J}\hat{p}) \rangle - 2ip\langle \hat{p}\hat{J} + \hat{J}\hat{p} + \hbar\hat{J} \rangle - 2i\bar{J}\langle \hat{J}^2 \rangle \\
&\quad - iJ\langle \hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J} + 4\hat{p}(\hat{p} + \hbar/2) \rangle + 2iJ^2\bar{J} + 4ip(p + \hbar/2)J \\
&= 6iG^{ppJ} + 8i(p + \hbar/2)G^{pJ} + 2iJG^{pp} - 2i\bar{J}G^{JJ} - 2iJG^{JJ} + 2ip^2J - 2iJ^2\bar{J} \\
&\quad + 2i\hbar pJ \\
&= 6iG^{ppJ} + 8i(p + \hbar/2)G^{pJ} - 2i\bar{J}G^{JJ} - i\hbar^2J,
\end{aligned}$$

$$\begin{aligned}
\{G^{pJ}, G^{p\bar{J}}\} &= \frac{1}{4i\hbar} \langle [\hat{p}\hat{J} + \hat{J}\hat{p}, \hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}] \rangle - \frac{1}{2i\hbar} p \langle [\hat{J}, \hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}] \rangle - \frac{1}{2i\hbar} J \langle [\hat{p}, \hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}] \rangle \\
&\quad - \frac{1}{2i\hbar} p \langle [\hat{p}\hat{J} + \hat{J}\hat{p}, \hat{J}^\dagger] \rangle - \frac{1}{2i\hbar} \bar{J} \langle [\hat{p}\hat{J} + \hat{J}\hat{p}, \hat{p}] \rangle + \{pJ, p\bar{J}\} \\
&= \frac{1}{4} i \langle 8\hat{p}^3 + \hat{p}(\hat{J}\hat{J}^\dagger + 2\hat{J}^\dagger\hat{J}) + (\hat{J}\hat{J}^\dagger + 2\hat{J}^\dagger\hat{J})\hat{p} + \hat{J}\hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p}\hat{J} + 4\hbar\hat{p}^2 \rangle \\
&\quad - ip\langle \hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J} + 4\hat{p}^2 + 2\hbar\hat{p} \rangle - \frac{1}{2} iJ\langle \hat{p}\hat{J}^\dagger + \hat{J}^\dagger\hat{p} \rangle - \frac{1}{2} i\bar{J}\langle \hat{p}\hat{J} + \hat{J}\hat{p} \rangle \\
&\quad + 2ipJ\bar{J} + 2ip^2(p + \hbar/2) \\
&= 4iG^{ppp} + i(8p + 3\hbar)G^{pp} - 2ipG^{J\bar{J}} - iJG^{p\bar{J}} - i\bar{J}G^{pJ} + 2ip^3 - 2ipJ\bar{J} \\
&\quad + 2i\hbar p^2 + \frac{3}{2}i\hbar^2p + \frac{1}{4}i\hbar^3 \\
&= 4iG^{ppp} + 6i(p + \hbar/2)G^{pp} - iJG^{p\bar{J}} - i\bar{J}G^{pJ} + \frac{1}{2}i\hbar^2p + \frac{1}{4}i\hbar^3
\end{aligned}$$

and

$$\begin{aligned}
\{G^{JJ}, G^{\bar{J}\bar{J}}\} &= \frac{1}{i\hbar} \langle [\hat{J}^2, (\hat{J}^\dagger)^2] \rangle - \frac{2}{i\hbar} J \langle [\hat{J}, (\hat{J}^\dagger)^2] \rangle - \frac{2}{i\hbar} \bar{J} \langle [\hat{J}^2, \hat{J}^\dagger] \rangle + \{J^2, \bar{J}^2\} \\
&= 2i\langle \hat{J}\hat{p}\hat{J}^\dagger + \hat{J}\hat{J}^\dagger\hat{p} + \hat{p}\hat{J}^\dagger\hat{J} + \hat{J}^\dagger\hat{p}\hat{J} + \hbar(\hat{J}\hat{J}^\dagger + \hat{J}^\dagger\hat{J}) \rangle - 4iJ\langle \hat{J}^\dagger\hat{p} + \hat{p}\hat{J}^\dagger + \hbar\hat{J}^\dagger \rangle \\
&\quad - 4i\bar{J}\langle \hat{J}\hat{p} + \hat{p}\hat{J} + \hbar\hat{J} \rangle + 8i(p + \hbar/2)J\bar{J} \\
&= 8iG^{ppp} + 16i(p + \hbar/2)G^{pp} + 8i(p + \hbar/2)G^{J\bar{J}} - 8iJG^{p\bar{J}} \\
&\quad - 8i\bar{J}G^{pJ} + 4i\hbar^2p + 2i\hbar^3.
\end{aligned}$$

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